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**DELIMITACIÓN DE CATEGORÍAS  
CIENTÍFICAS EN BASES DE DATOS  
MULTIDISCIPLINARES: NANOCIENCIA Y  
NANOTECNOLOGÍA COMO ESTUDIO DE  
CASO**

**SUBJECT AREAS DELINEATION IN  
MULTIDISCIPLINARY DATABASES:  
NANOSCIENCE AND NANOTECHNOLOGY AS  
CASE STUDY**

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## Resumen

Para la gestión de la política científica, la evaluación de la ciencia es crucial a la hora de establecer prioridades y nuevos retos que sobrepasen las fronteras del conocimiento en investigación y desarrollo. Un paso previo a la evaluación de las disciplinas científicas<sup>1</sup> es su adecuada delimitación temática, que consiste en asignar revistas o publicaciones a categoría científicas. Sin embargo, la delimitación de campos de conocimiento sigue siendo una tarea compleja, especialmente para disciplinas emergentes. En consecuencia, es importante explorar y combinar los distintos enfoques metodológicos para tener una representación lo más fiable y exhaustiva posible de la delimitación y el desarrollo de las disciplinas científicas. Este proceso puede ser útil para ayudar en la toma de decisiones en la gestión de la investigación.

El conocimiento generado mediante la investigación y la innovación en muchas disciplinas científicas emergentes, como la robótica o la biología sintética, presenta un gran atractivo para el desarrollo de los países. Este es el caso de Nanociencia y Nanotecnología (NST), un dominio científico con un enorme potencial económico. Conocer las principales líneas de investigación y la especialización temática de países o instituciones puede repercutir positivamente en el diseño de agendas científicas en un entorno competitivo a nivel global.

Esta tesis doctoral estudia la delimitación de categorías científicas, que consiste en asignar revistas o publicaciones a un campo temático. El objetivo es conocer la problemática inherente a esta clasificación y explorar otros enfoques y metodologías que sean útiles para el propio campo de conocimiento en el que se enmarca y, a su vez, mejore la capacidad de realizar diagnósticos basados en el desempeño científico de una disciplina.

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<sup>1</sup> Los términos dominio científico, campo de conocimiento y disciplina científica se usan indistintamente.

Para tal fin, se llevaron a cabo una serie de estudios de caso basados en el análisis de la producción científica de NST indexada en las bases de datos de carácter multidisciplinar e internacional Web of Science (WoS) y Scopus. Tras la descarga de las publicaciones de la categoría de WoS *Nanoscience & Nanotechnology*, se aplicaron análisis de citas y de copalabras para determinar su estructura intelectual y cognitiva. En segundo lugar, se diseñó una estrategia de búsqueda basada en términos de NST para recuperar la colección de documentos indexada en WoS y Scopus (2008-2015). Seguidamente, se experimentó con tres aproximaciones para poder comparar la delimitación de campos de conocimiento entre ellas: 1) a nivel de categoría temática, utilizando la categoría temática de WoS *Nanoscience & Nanotechnology*; 2) a nivel de revistas, desarrollando una metodología para la delimitación de categorías; y 3) a nivel de publicaciones, empleando la metodología desarrollada por el Centre for Science and Technology Studies (CWTS). La validación, mediante la consulta a expertos, ayudó a determinar los valores de precisión y exhaustividad para cada una de las aproximaciones. En tercer lugar, se aplicó el análisis de copalabras, utilizando *author keywords* e *indexed keywords* de las publicaciones de NST indexadas en Scopus (2010-2014-2018) para un conjunto de países (Alemania, Francia y España) y se calcularon indicadores de especialización temática, tanto a nivel de producción como a nivel de palabras clave. Esto permitió la distinción de los patrones de publicación y de especialización en NST y su comparación en los países objeto de estudio.

Los resultados del análisis combinado de copalabras y *clustering* muestran un total de 7 frentes de investigación: *Microingeniería Electrónica y Procesos Top-down*, *Síntesis de Nanomateriales y Procesos Bottom-up*, *Características Físicas de los Nanomateriales*, *Características Mecánicas de los Nanomateriales*, *Óptica y Electrónica*, *Biología y Biomedicina: Biodetección*, *Biología y Biomedicina: Biología Terapéutica y Electrónica Orgánica*, aunque los más dinámicos fueron *Microingeniería Electrónica y Procesos Top-Down*, *Síntesis de Nanomateriales y Procesos*

*Bottom-up y Biotecnología y Biomedicina.* El estudio de las citas reveló que la estructura intelectual de la NST se compone de 7 temáticas claramente definidas. La investigación de *Nanomateriales de Carbono* destacó como una de las áreas más influyentes y prolíficas en el desarrollo de la NST.

El análisis de los enfoques metodológicos empleados para la delimitación de la NST desveló que los mejores resultados, en cuanto a precisión y exhaustividad, procedían de la delimitación a nivel de revistas, seguida de la delimitación a nivel de publicaciones. Sin embargo, estos datos deben ser interpretados con cautela, pues el nivel de desacuerdo entre los expertos consultados en la validación fue notable.

El análisis de la especialización temática desveló un mayor esfuerzo en la investigación aplicada que en la investigación básica a nivel global. Paralelamente, la especialización a nivel de palabras clave reveló poca especialización en todos los frentes de investigación para España, Alemania y Francia, lo que sugiere que el desarrollo de esta disciplina es más fuerte en otros países. Sin embargo, para los valores calculados atendiendo al número de ocurrencias, España presenta mejores resultados que Alemania y Francia en la investigación en *Biotecnología y Biomedicina y Características Físicas y Mecánicas de los Nanomateriales.*

Esta investigación proporciona a los académicos, investigadores y gestores de investigación resultados que pueden ser de gran valor para facilitar la comprensión de dominios científicos emergentes y/o multi/interdisciplinares, así como sus relaciones con otras áreas de investigación. Estos hallazgos pueden complementar la información necesaria para trazar acciones en torno a la clasificación de la literatura en bases de datos multidisciplinares y al uso que se hace de la especialización temática como elemento clave en la gestión de la investigación.

## **Abstract**

For the management of scientific policy, science evaluation is essential when establishing priorities and new challenges that go beyond the frontiers of knowledge in research and development. A previous step to the evaluation of scientific disciplines<sup>2</sup> is their adequate delineation that consists of assigning journals or publications to subject categories. However, field delineation remains a complex task, especially for emerging disciplines. Consequently, it is important to explore and combine the different methodological approaches in order to have as a reliable and exhaustive representation as possible of the delineation and development of scientific disciplines. This process can be useful in aiding decision-making in research management.

The knowledge generated through research and innovation in many emerging scientific disciplines, such as robotics or synthetic biology, offers a great interest for the development of countries. This is the case with Nanoscience and Nanotechnology (NST), an emerging scientific domain with enormous economic potential. To know main research fronts and thematic specialization of countries or institutions can have a positive impact on the design of scientific agendas in a globally competitive environment.

This dissertation studies scientific category delineation that consists of assigning journals or publications to a thematic area. The objective is to know the inherent problems in that classification and, if necessary, explore other approaches and methodologies that are useful for the knowledge field in which it is framed and, in turn, improve the ability to make diagnoses based on the scientific performance of a discipline.

For this purpose, a series of case studies were conducted on the analysis of the scientific output of NST indexed in the multidisciplinary and international databases Web of Science (WoS) and Scopus. After downloading the

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<sup>2</sup> The terms scientific domain, knowledge field, and scientific discipline are interchangeably used.

publications from the WoS Subject Category Nanoscience & Nanotechnology, citation and co-word analysis were applied to determine the intellectual and cognitive structure. Second, a lexical query based on NST terms was designed to retrieve the documents indexed in WoS and Scopus (2008-2015). Then, we experimented with three approaches that so compare them for the knowledge fields delineation: 1) at the subject category level, using the WoS Subject Category Nanoscience & Nanotechnology; 2) at the journals level, developing a methodology for categories delineation; and 3) at the publications level, using the methodology developed by the Center for Science and Technology Studies (CWTS). The validation, through expert consultation, helped determine the precision and recall indicators for each approach. Third, the co-words analysis was applied by using author keywords and indexed keywords of NST publications indexed in Scopus (2010-2014-2018) from a countries set (Germany, France and Spain). Afterwards, thematic specialization indicators were calculated, both at production level as well as at the keyword level. This made possible to distinguish the publication patterns and specialization in NST and their comparison in the countries under study.

The outcomes of the combined co-words and clustering analysis identified a total of 7 research fronts: *Microelectronics Engineering and Top-down Processes*, *Synthesis of Nanomaterials and Bottom-up Processes*, *Physical Characteristics of Nanomaterials*, *Mechanical Characteristics of Nanomaterials*, *Optics and Electronics*, *Biotechnology and Biomedicine: Biodetection*, *Biotechnology and Biomedicine: Therapeutic Biomedicine* and *Organic Electronics*. The most representative research fronts and the ones with the greatest dynamics in the development of NST were *Microelectronics Engineering and Top-down Processes*, *Synthesis of Nanomaterials and Bottom-up Processes* and *Biotechnology and Biomedicine*. Citation analysis revealed that the intellectual structure of NST is made up of seven clearly defined topics. *Carbon Nanomaterials* research stood out as one of the most influential and prolific areas in the development of NST.

The analysis of the methodological approaches used for the NST delineation revealed that the best results, in terms of precision and recall, came from delineation at the journal level, followed by delineation at the publication level. However, these data have to be interpreted with caution, since the level of disagreement between the consulted experts in the validation was notable.

The topic specialization analysis showed a greater effort in applied research than in basic research. At the same time, specialization at keyword level revealed slightly specialization on all research fronts for Spain, Germany, and France. This fact suggests that the development of this discipline is stronger in other countries. However, for the values calculated according to the number of occurrences, Spain presents better results than Germany and France in *Biotechnology and Biomedicine* and *Physical and Mechanical Characteristics of Nanomaterials*

This research provides academics, researchers, and research managers with results that can be a valuable tool to facilitate the understanding of emerging scientific and / or multi/interdisciplinary domains, as well as their relationships with other research areas. These findings can complement the information needed to outline actions around the classification in multidisciplinary databases and the usage made of this thematic specialization as a key element in research management.



## Estructura de la tesis

Esta tesis se presenta bajo la modalidad de compendio de publicaciones científicas, atendiendo al listado de revistas incluidas en el *Journal Citation Reports* de la Web of Science, según lo dispuesto en el reglamento del Programa de Doctorado de la Universidad de Granada<sup>3</sup>. Las publicaciones científicas que conforman esta tesis doctoral dan respuesta a las preguntas de investigación sobre cómo determinar la estructura intelectual y cognitiva de un dominio científico; qué aproximaciones metodológicas debemos considerar para su delimitación; y cómo se puede explorar de manera combinada la estructura cognitiva y la especialización de un dominio científico para conocer las fortalezas de cada país en determinadas líneas de investigación.

A continuación se resumen las publicaciones que componen esta tesis:

1. Muñoz-Écija, T., Vargas-Quesada, B., & Chinchilla-Rodríguez, Z. (2017). Identification and visualization of the intellectual structure and the main research lines in nanoscience and nanotechnology at the worldwide level. *Journal of Nanoparticle Research*, 19(2), 62.  
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Los estudios cuantitativos de la ciencia son comúnmente utilizados para estudiar dominios científicos o temáticas específicas y servir de herramienta de análisis en el contexto de la gestión y la política científica. Sin embargo, la ciencia es cada vez más interdisciplinar, lo cual acarrea cierta complejidad en su análisis. En este trabajo se identifica y explora la estructura intelectual y cognitiva del dominio científico Nanociencia y Nanotecnología mediante el uso de técnicas bibliométricas y de visualización, en concreto a través de mapas de la ciencia. Partiendo de las publicaciones de la Web of Science (WoS), se han podido identificar tanto los orígenes de la producción científica en este campo de conocimiento como las publicaciones más influyentes en su desarrollo científico, mediante el análisis de citación directa y la

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<sup>3</sup> [https://secretariageneral.ugr.es/bougr/pages/bougr153/\\_doc/doctorado/%21](https://secretariageneral.ugr.es/bougr/pages/bougr153/_doc/doctorado/%21)

visualización de histogramas. Asimismo, se ha logrado identificar las principales áreas temáticas dentro de la NST, mediante el análisis de copalabras. A partir de estos resultados se reafirma que la NST es una disciplina incipiente, en constante desarrollo y con un marcado carácter interdisciplinar, alimentada principalmente por la física, la química, la ciencia de los materiales o la ingeniería. La aplicación de estas metodologías muestra un análisis a gran escala de las áreas de investigación de NST y cómo las líneas de investigación han cambiado con el tiempo. Su principal contribución al campo de los estudios cuantitativos de la ciencia es el período de tiempo analizado a nivel mundial y que la combinación de metodologías es extrapolable a otras disciplinas científicas y niveles de agregación (nacional, regional, institucional) para determinar la estructura intelectual y cognitiva.

2. Muñoz-Écija, T., Vargas-Quesada, B., & Chinchilla-Rodríguez, Z. (2019). Coping with methods for delineating emerging fields: Nanoscience and nanotechnology as a case study. *Journal of Informetrics*, 13(4), 100976. <https://doi.org/10.1016/j.joi.2019.100976>

La delimitación de dominios científicos juega un papel importante en los estudios cuantitativos, aunque es una tarea compleja. En este trabajo se ha destacado la problemática implícita en la delimitación de dominios científicos, especialmente cuando son emergentes e interdisciplinarios, como es la NST. Para ello, se recuperó la producción científica relacionada con NST y se aplicaron tres enfoques diferentes para delinear un campo de conocimiento que comprenden tres niveles dispares de agregación: categoría temática, revistas y publicaciones. Posteriormente, se elaboró una encuesta para recabar la opinión de los expertos y validar los resultados. Para comparar los diversos enfoques aplicados se calcularon las medidas de Precisión y Exhaustividad. Como resultado, se ha confirmado la complejidad inherente en la delimitación de dominios científicos, tanto a nivel cuantitativo como cualitativo, incluso cuando los expertos corroboran los resultados.

3. Muñoz-Écija, T., Vargas-Quesada, B., & Chinchilla-Rodríguez, Z. (2022). Unveiling cognitive structure and comparative advantages of countries in knowledge domains. *Journal of Information Science*. <https://doi.org/10.1177/01655515221084607>

El mapeo y descripción de la estructura de un determinado dominio científico, así como la caracterización de los perfiles de especialización, permiten una mejor comprensión de su evolución, así como de sus fortalezas y debilidades. La identificación de perfiles de especialización a diferentes niveles —global, nacional o regional— puede servir de ayuda en la toma de decisiones con respecto a la gestión de la investigación. Este artículo analiza la evolución de la estructura cognitiva de un campo de conocimiento a nivel de país, con el objetivo de caracterizar y rastrear su desarrollo y determinar la competitividad en términos de especialización en investigación. A partir de un conjunto de datos extraídos de la base de datos Scopus, se aplica el análisis de copalabras para visualizar su estructura cognitiva y estudiar el grado de especialización basado en artículos y palabras clave de NST, en tres países miembros de la Unión Europea: Alemania, España y Francia. Los resultados revelan que la investigación de NST tiende a centrarse en nanoaplicaciones y nanodispositivos. Según el índice de actividad de palabras clave, los países estudiados centran su especialización en la investigación electrónica, biotecnológica y biomédica, mostrando algunos de ellos una ventaja más competitiva en el ámbito global. Como colofón, se describen las implicaciones que podrían contribuir a la toma de decisiones en materia de gestión y diseño de agendas de investigación.

## **Parte I: Aspectos generales de la investigación**

### **Capítulo 1. Introducción**

Tras reconocer la importancia y repercusión de la aplicación del conocimiento científico a la solución de problemas durante la Segunda Guerra Mundial, la gestión de la política científica es considerada un asunto de suma importancia por su gran repercusión en el bienestar y desarrollo de un país, y por el enorme potencial que supone la competitividad en ciencia y tecnología de un Estado (Bush, 1945). Así, la evaluación de la ciencia se hace imprescindible para el diseño de las políticas científicas de los gobiernos, a la hora de valorar y establecer prioridades en investigación y desarrollo en áreas competitivas, lo cual tiene una gran influencia en el progreso económico y bienestar social de los países (Gobierno de España, 2019).

Los actuales sistemas de financiación de la Unión Europea (UE) en Investigación, Desarrollo e Innovación (I+D+i) tienen entre sus objetivos impulsar políticas orientadas a los retos de la sociedad, además de promover estrategias de especialización inteligente en investigación e innovación orientadas a optimizar el uso de los fondos (European Commission et al., 2021). La principal finalidad de estas estrategias es disminuir la diferencia en competitividad entre la UE y Estados Unidos. Este concepto de especialización inteligente hace referencia a las prioridades, retos y necesidades que los territorios deben establecer para el desarrollo, basado en el conocimiento generado a través de la investigación y la innovación (Hegyí et al., 2021). La estrategia de especialización inteligente también es impulsada por organizaciones supranacionales como la OCDE, con una combinación de políticas industriales, educativas y de innovación para sugerir que los países o regiones identifiquen y seleccionen un número limitado de áreas prioritarias para inversiones basadas en el conocimiento, centrándose en sus fortalezas y ventajas comparativas (OECD, 2013). De ahí que los diferentes territorios tengan la necesidad de determinar cuáles son sus

fortalezas y debilidades e identificar líneas emergentes de interés en ámbitos competitivos y generadores de desarrollo en un contexto global, además de dotarse de sistemas de supervisión y evaluación (Guzzo & Gianelle, 2021; Zacca-González et al., 2018).

Ante este panorama, para el diseño de agendas científicas sólidas e incluyentes, los Estados deben dotarse de datos y herramientas que les permitan realizar un seguimiento de la investigación para respaldar la toma de decisiones. Los estudios cuantitativos de la ciencia son una de las herramientas utilizadas en la monitorización de los resultados de la actividad científica. Los resultados de estos estudios ayudan en la toma de decisiones, ofreciendo información objetiva para optimizar la distribución de los recursos, definir programas de movilidad internacional, establecer redes de colaboración, detectar clústeres científicos-tecnológicos, fomentar la investigación en temas de vanguardia y facilitar la incorporación de los resultados de investigación a la industria y, finalmente, a la sociedad (Chinchilla-Rodríguez & De Moya-Anegón, 2007).

Los frentes de investigación emergentes que surgen dentro de un campo de conocimiento generan un gran atractivo para los distintos estados o países. En este sentido, la aplicación de métodos bibliométricos, junto con el análisis de redes para el estudio de la producción científica, son frecuentemente utilizados con el fin de identificar, delimitar y rastrear el desarrollo y la trayectoria científica de los campos emergentes de la manera más precisa y exhaustiva posible (Liang et al., 2021; Wang, 2018; Shapira et al., 2017; Glänzel, 2012). Sin embargo, estas tareas no resultan sencillas, aunque existen una gran cantidad de enfoques desde los que pueden ser abordadas, especialmente cuando los dominios científicos a delimitar son bastante multi/interdisciplinarios e inestables (Finardi & Lamberti, 2021; Porter & Youtie, 2009a; Schummer, 2004).

La mejor forma de comprender la información de un determinado campo o disciplina científica es estudiando la forma en que los miembros de la comunidad que la componen se relacionan y comunican entre sí por medio de su producción científica, que no es más que un reflejo de su situación intelectual, económica, social, etc. A este tipo de enfoque se le conoce como Análisis de Dominios Científicos (Vargas-Quesada & de Moya-Anegón, 2007; Hjørland & Albrechtsen, 1995). En este contexto se enmarca el estudio de la producción en NST, un campo científico que ha sido definido como una de las áreas estratégicas por su gran potencial económico a nivel mundial (Wood et al., 2003). Buena prueba de ello ha sido su incorporación en los programas nacionales de I+D+i, así como la inversión destinada a investigación desde el año 2000, cuando Estados Unidos creó la *National Nanotechnology Initiative*. Este hecho provocó la reacción en cadena por parte de otros países como China o Japón, que priorizó la investigación de NST (Shapira & Wang, 2010).

A su vez, su gran potencial económico radica en los beneficios para el desarrollo que presentan muchas de las aplicaciones de NST, las cuales están marcando el rumbo de la investigación científica. Shapira y colaboradores (2011) enfatizan que antes de avanzar en la fase de comercialización y crecimiento económico, existe una fase previa de producción científica. La presencia de inversión económica para la producción científica resulta vital, pero ¿qué ocurre cuándo los países cuentan con escasos recursos económicos para la investigación? ¿Cómo puede desarrollarse la investigación de un país con respecto a sus posibles competidores o colaboradores? Las respuestas a estas preguntas podemos encontrarlas en la identificación de temas estratégicos que necesitan una inversión para favorecer el desarrollo y crecimiento de los países (Pinto & Teixeira, 2020), atendiendo a su capacidad de absorción de conocimiento e innovación (Fagerberg & Srholec, 2017b; Solarin & Yen, 2016; Fagerberg & Srholec, 2008; Freeman, 2002).

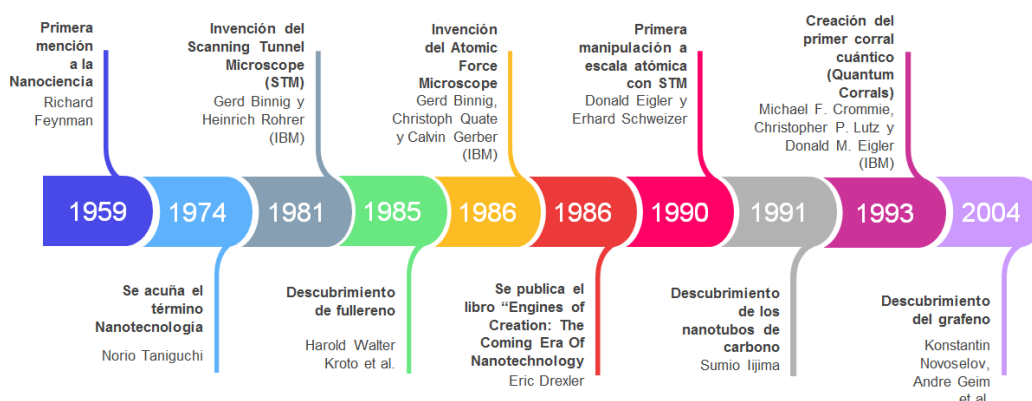
## 1.1. Delimitación del estudio

En esta tesis doctoral se delimita un dominio científico emergente y bastante dinámico, como es Nanociencia y Nanotecnología, a través del análisis de la producción científica indizada en Scopus y Web of Science. El objetivo es estudiar las principales líneas de investigación y sus patrones de comportamiento, con el fin de delimitar su producción e identificar líneas emergentes de interés en ámbitos competitivos y generadores de desarrollo en un contexto global.

La NST puede ser definida como la disciplina científica que comprende el estudio, diseño, creación, síntesis, manipulación y aplicación de materiales, dispositivos y sistemas funcionales mediante el control del material a nanoescala; así como la explotación de fenómenos y propiedades del material a escala nanométrica. Además podemos definir la investigación en nanociencia como aquella investigación procedente de la convergencia de física, ciencia de los materiales y biología, que se ocupa de la manipulación de materiales a escalas molecular y atómica (Porter & Youtie, 2009a); mientras que la investigación en nanotecnología es la procedente de observar, medir, manipular, ensamblar, controlar y fabricar materia a escala nanométrica (Bayda et al., 2020).

La Figura 1 muestra cronológicamente los hitos científicos más relevantes de la NST. Se la considera una ciencia relativamente joven, ya que aparece en la segunda mitad del siglo XX, cuando Richard P. Feynman (1960) se refirió a las posibilidades que ofrece la manipulación de material a escala atómica. No fue hasta la década de los 80 cuando la producción comenzó a aumentar a raíz del descubrimiento microscopio de efecto túnel (Binnig & Rohrer, 1983), el cual permitió a la comunidad científica el desarrollo de nuevos materiales e instrumentos. No obstante, fue a partir del año 2000 cuando el crecimiento exponencial de su producción se hizo mucho más notable (Grieneisen & Zhang, 2012). Uno de los avances científicos que contribuyó a este aumento

fue el descubrimiento del grafeno (Novoselov et al., 2004), que abrió un sinfín de oportunidades para la investigación e innovación en NST.



**Figura 1.** Principales hitos en Nanociencia y Nanotecnología

Este campo temático ha sido considerado durante los últimos veinte años como una de las bases de transformación científica y económica en el mundo actual, convirtiéndose en una de las áreas estratégicas por su gran potencial. La investigación en NST, así como los productos y servicios procedentes de dicha investigación, suponen importantes beneficios económicos y sociales (Sargent, 2016). La revolución nanotecnológica ha proporcionado innumerables avances en medicina, energía, electrónica, agricultura, medio ambiente, etc., al mismo tiempo que pone de manifiesto cuestiones éticas de su aplicación relacionadas con los peligros ambientales y para la salud (Babatunde et al., 2020).

De las enormes posibilidades que presenta la NST surgió una línea de investigación guiada por la necesidad de evaluar el impacto económico, con el objetivo de estimular las decisiones políticas y el apoyo público en forma de inversión (Gorsuch & Link, 2018). La inversión pública en este dominio científico es fundamental para adquirir conocimientos a través de la investigación, apoyar la competitividad, el crecimiento económico, comercializar nuevas tecnologías y productos y, por último, abordar problemas sociales (Liu & Porter, 2020; Roco et al., 2011; Roco & Bainbridge, 2005). Sin el apoyo a la investigación básica en NST resulta difícil cosechar



éxitos, pues se precisa de tiempo entre inversión inicial y resultados, en este caso en forma de descubrimientos y desarrollos (Weiss, 2021).

El carácter multidisciplinar y la diversidad de la NST determinan patrones de comunicación propios, que es importante entender para tener una idea más holística de su desarrollo y sus implicaciones para el diseño de agendas en política científica, la financiación, la gestión de la investigación y la transferencia eficaz de conocimientos (Porter & Youtie, 2009b). La identificación de estos patrones de comunicación en el área permite mejorar aquellos aspectos que puedan ser básicos para su desarrollo y/o reforzar lo que está funcionando bien, para que su impacto económico y social sea diverso e inclusivo a nivel de territorios.

Debido a su trascendencia, disponer de herramientas que permitan delimitar el ámbito científico de la NST para caracterizar el desempeño de la investigación científica, con la integración de técnicas cuantitativas de la ciencia y fuentes de información internacionales, posibilitará adquirir nuevos conocimientos y repercutirá en la capacidad informativa y analítica de la investigación científica en NST.

Por tanto, la contribución fundamental de esta tesis es proporcionar un instrumento que permita analizar el desarrollo de la NST, sus dinámicas y el potencial que presenta para el futuro de los territorios, desde el punto de vista del análisis cuantitativo de la producción científica. Asimismo, la información resultante puede facilitar el desarrollo de futuros procesos de delimitación temática y ayudar en el diseño y gestión de agendas y políticas científicas, teniendo en cuenta los principales frentes de investigación y la especialización temática de los territorios.

## **1.2. La importancia de la Nanociencia y Nanotecnología**

En Europa, la NST forma parte de la política de I+D+i, siendo un elemento clave en la política industrial europea gracias a la innovación de productos

para todos los sectores industriales. Desde 2002, varias han sido las políticas europeas encaminadas al desarrollo de la investigación e innovación en NST. La Unión Europea ha destinado millones de euros al gasto en I+D en NST a través de los diferentes Programas Marco -FP6 y FP7-, el Programa Horizonte 2020 (H2020) y el Programa Horizonte Europa 2021-2027. Uno de los objetivos específicos del H2020 era “garantizar el liderazgo de la Unión Europea en este mercado global en auge, mediante la estimulación de avances científicos y tecnológicos y de la inversión en nanotecnologías, así como su asimilación en sectores, a través de una amplia gama de aplicaciones en productos de alto valor añadido y servicios competitivos” (Fundación Española para la Ciencia y la Tecnología, 2018).

Debido a la variedad de campos de aplicación de la NST resulta complicado poder medir su impacto. A nivel microeconómico, es difícil hacer estimaciones por la transversalidad de la NST. A nivel macroeconómico, la UE estima un aumento de los productos e infraestructura nanotecnológicas en diferentes sectores como el fotónico, el energético, el transporte, el sanitario o la construcción para los años venideros (European Commision, 2013).

En España, la Nanociencia y Nanotecnología fue incluida en 2006 como una de las líneas estratégicas dentro de Programa CENIT (Centro para el Desarrollo Tecnológico e Industrial)<sup>4</sup>. Este programa tuvo gran impacto en su desarrollo en España, estimulando la cooperación público-privada en investigación industrial y generando los consorcios DOMINO y NanoFarma.

Otra de las iniciativas llevadas en cabo fue el programa CONSOLIDER, pilar estratégico del Programa Ingenio 2010, cuyo propósito era alcanzar la excelencia en la investigación. Para ello, se proponía incrementar la

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<sup>4</sup> Centro para el Desarrollo Tecnológico e Industrial (España). (2006). Programa CENIT. Disponible en: <http://www.cdti.es/index.asp?MP=4&MS=0&MN=1&textobuscado=cenit&tipo=1&TR=A&IDR=38&tipoO=Contenido&id=50&xtmc=cenit&xtcr=7>

cooperación entre grupos de investigación y financiar actuaciones de carácter estratégico, basadas en actividades científicas. Estas actividades iban encaminadas a promover un avance significativo en el estado del conocimiento o a establecer líneas de investigación originales situadas en lo que se denomina frontera del conocimiento. Su aplicación dio lugar a diferentes iniciativas como NANOBIO MED y CIC NanoGUNE en 2006; o NANOMOL, NANOSELECT y Nanolight.es en 2007.

Desde 2010 se desarrollaron varias estrategias para la financiación de proyectos de I+D, tanto para el sector privado como para el público, como el Programa CIEN (Programa Estratégico de Investigación Empresarial Nacional) o el apoyo y acreditación de Centros y Unidades de Excelencia Severo Ochoa y María de Maeztu.

Por otro lado, la Acción Estratégica de Nanociencia y Nanotecnología, Nuevos Materiales y Nuevos Procesos Industriales<sup>5</sup> tenía como objetivo mejorar la competitividad de la industria española mediante la implementación de conocimiento y el desarrollo de nuevas aplicaciones en NST. Esta Acción Estratégica tuvo continuidad en el Plan Nacional de I+D+i 2008-2011 y, actualmente, se enmarca dentro de las Acciones Estratégicas definidas en la Estrategia Española de Ciencia, Tecnología e Innovación 2021-2027 y articuladas en el Plan Estatal de Investigación Científica, Técnica y de Innovación 2021–2023. Tales acciones estratégicas tienen como objetivo cohesionar políticas sectoriales en I+D+i, así como guiar la visión estratégica y el enfoque temático de los Programas y Subprogramas que componen el Plan Estatal. Por tanto, la aplicación de NST en lo referido a salud,

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<sup>5</sup> Ministerio de Educación y Ciencia (España). (2004). *Acción Estratégica de Nanociencia y Nanotecnología, Nuevos Materiales y Nuevos Procesos Industriales*. Disponible en: <https://sede.educacion.gob.es/publiventa/d/20560/19/1>

transformación digital, industria, defensa, cambio climático, energía, movilidad, etc. es considerada una de las áreas de trabajo fundamentales<sup>6</sup>.

España cuenta, por el momento, con diecisiete centros I+D+i y alrededor de 105 empresas dedicados a la Nanociencia y Nanotecnología o a algunas de sus especialidades. Madrid, País Vasco y Cataluña son las comunidades autónomas con mayor número de empresas especializadas en NST, aunque no superan el 47% sobre el total de empresas en España (Phantoms Foundation, 2017). Además, existen otros muchos centros de I+D y unidades de investigación que realizan actividades relacionadas con Nanociencia y Nanotecnología, aunque no se definan como tal (Fundación Española para la Ciencia y la Tecnología, 2018).

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<sup>6</sup> Ministerio de Ciencia e Innovación (España). (2021). *Plan Estatal de Investigación Científica, Técnica y de Innovación 2021-2023*. Disponible en: <https://www.ciencia.gob.es/InfoGeneralPortal/documento/e1f1deb1-7321-4dd9-b8ca-f97ece358d1c>

## Capítulo 2. Antecedentes

### 2.1. Evaluación cuantitativa en Nanociencia y Nanotecnología

La cienciometría es la disciplina que estudia los aspectos cuantitativos de la literatura científica y tecnológica sobre el desarrollo de la ciencia como proceso informativo (Van Raan, 1997). Gracias a ella se generan datos e indicadores para, entre otras cosas, monitorear el desempeño científico, seleccionar prioridades de investigación y estudiar las relaciones entre ciencia y economía o ciencia y sociedad, lo cual permite el desarrollo de políticas científicas (Vinkler, 2010).

De acuerdo al portal especializado StatNano<sup>7</sup>, la producción científica española indizada en la categoría Nanoscience & Nanotechnology de la WoS entre los años 2000 y 2020 fue de 59.753 publicaciones, representando un 3,1% de la producción a nivel mundial en esta área. En 2020, España ocupaba el puesto 12 del ranking mundial en artículos científicos indizados en WoS (5.472 publicaciones sobre un total de 211.700); el puesto 11, con 3.327 publicaciones (101.763 publicaciones a nivel mundial) en revistas de primer cuartil indexadas en el *Journal Citation Reports*. De estas 3.327, 1.037 están publicadas en las revistas con el factor de impacto más alto. En general, España ha mostrado un crecimiento firme y constante del número de publicaciones, gran parte de ellas en revistas de alto impacto (78%), consideradas altamente citadas (18,5%) y elaboradas en colaboración internacional (60%). De igual modo, la media de impacto normalizado anual indicó una tendencia ascendente, llegando a superar a la media mundial (Fundación Española para la Ciencia y la Tecnología, 2018). Respecto al índice h para el año 2020, España ocupó el puesto 23 con un valor de 27, correspondiendo el mayor valor a los Estados Unidos, con un índice h de 72.

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<sup>7</sup> <https://statnano.com>

A nivel mundial, los estudios cuantitativos de la ciencia han sido una de las herramientas que han facilitado caracterizar los principales autores y países productores (Kostoff et al., 2007b), estudiar las dinámicas de sus temas de investigación y las redes de colaboración (Arora et al., 2013; Zheng et al., 2014) o el impacto económico y social con la evaluación de políticas y patentes (Chen et al., 2013; Beaudry & Allaoui, 2012; Shapira et al., 2011).

Diversas técnicas bibliométricas han contribuido a estudiar el desarrollo de algunos subdominios científicos que componen la NST, como, por ejemplo, investigaciones que examinaban nanotubos de carbono (Munoz-Sandoval, 2013), nanoenergía (Guan & Liu, 2014; Menéndez-Manjón et al., 2011), materiales nanoluminiscentes (Zhao et al., 2020), diferentes propiedades de las nanopartículas (Yang & Ho, 2019; Liu et al., 2016), nanotoxicología (Tang et al., 2018; Ostrowski et al., 2009), sistemas nanoelectromecánicos (Hu & Liu, 2015) y nanoburbujas (Zheng et al., 2016), por mencionar algunos casos.

Otros estudios emplearon técnicas bibliométricas para medir el desempeño científico de los países (Chinchilla-Rodríguez et al., 2018, 2016; Chen et al., 2013; Kostoff et al., 2007a); comparar países desarrollados y países en vías de desarrollo (Jafari & Zarghami, 2016); destacar la actividad y visibilidad en el panorama global de algunos países, entre ellos China (Tang & Shapira, 2011), Rusia (Terekhov, 2012), India (Chauhan, 2020) o países de América Latina (Invernizzi et al., 2015); evaluar la productividad, los temas de investigación dominantes y los patrones de difusión en Rusia, China e India (Liu et al., 2009); identificar nanomateriales y aplicaciones que suponen un riesgo para el medioambiente, a través de sus patentes (Leitch et al., 2012); o para identificar tendencias de crecimiento, temas de investigación, la evolución en la financiación de la *National Science Foundation* y las actividades comerciales de patentes de la USPTO (Huang et al., 2006).

### **2.1.1. Delimitación temática**

La delimitación temática, consistente en asignar revistas o publicaciones a categoría científicas, suele ser una de las primera tareas que se realizan antes de abordar el análisis cuantitativo de cualquier campo temático (Zhao, 2009). Es una tarea compleja debido al carácter multi, inter o transdisciplinar que adopta la ciencia en la actualidad, al generar vínculos con otras áreas de investigación (Sugimoto & Weingart, 2015). De manera que el proceso de delimitación de temáticas emergentes es todo un desafío, si se pretende con él una representación exhaustiva de toda la literatura indexada en una fuente de información o en la combinación de distintas fuentes de información bibliográficas (Vargas-Quesada et al., 2017; Milanez et al., 2016; Vargas-Quesada et al., 2010; Vargas-Quesada & de Moya-Anegón, 2007; Vargas-Quesada, 2005).

De hecho, una adecuada delimitación temática resulta fundamental a la hora de confeccionar herramientas confiables y sólidas para elaborar rankings y análisis de dominios científicos, resaltando su gran valor en el diseño de políticas científicas y procesos de evaluación científica (Gómez-Núñez, Vargas-Quesada, & de Moya-Anegón, 2016; Gómez-Núñez et al., 2014).

La jerarquía de las ciencias proporciona un marco para comprender la diversidad de un dominio científico, pues refleja el nivel de consenso académico y muestra dicotomías naturales-sociales (Fanelli & Glänzel, 2013). Esta jerarquía plasma cómo el consenso de la comunidad científica perteneciente a un dominio científico determinado se alcanza fácilmente a nivel central (donde las teorías o métodos están completamente aceptados), pero no a nivel fronterizo (donde se realiza la investigación) (Cole, 1983). El consenso puede involucrar no solo aspectos cognitivos o la complejidad de un dominio científico, sino también aspectos sociológicos. Por tanto, la definición de un dominio científico deriva tanto de su contenido científico como de la asociación e interacción (social, profesional o editorial) de sus investigadores. De hecho, la falta de cohesión en un dominio científico puede

considerarse como un factor para detectar un dominio científico emergente (Casadevall & Fang, 2015). Asimismo, delimitar dominios científicos se puede llevar a cabo a partir de técnicas empíricas y pragmáticas u otros procedimientos automatizados basados en estadísticas y métodos computarizados.

Desde el punto de vista de los estudios cuantitativos de ciencia y tecnología, son varios los modelos existentes para la delimitación temática. En primer lugar, los sistemas de clasificación diseñados por entidades como, por ejemplo, asociaciones profesionales, editores, instituciones o corporaciones. En segundo lugar, el uso de estrategias de búsquedas para la recuperación de información del dominio científico. Y, en tercer lugar, las técnicas de mapeo y agrupamiento (*clustering*).

### **2.1.2. Sistemas de clasificación**

Los sistemas de clasificación son considerados una herramienta esencial para estudiar la estructura y las dinámicas de un dominio científico (Zitt et al., 2005) y, generalmente, se han basado en la clasificación a nivel de revista (Gómez-Núñez et al., 2016; McCain, 2010; Leydesdorff, 2008; Leydesdorff & Cozzens, 1993) o en la clasificación a nivel de publicación (Sjögårde & Ahlgren, 2018; Boyack & Klavans, 2014; Waltman & van Eck, 2012). Un adecuado sistema de clasificación ayuda en tareas como la recuperación de la producción científica de un campo de conocimiento, la evaluación y comparación con otras disciplinas científicas o el estudio de la interdisciplinariedad del campo (Glänzel, 2015).

Aunque los esquemas de clasificación de categorías pueden definir un dominio científico a nivel meso, este tipo de delineación encuentra limitaciones a nivel micro, debido a las revistas multidisciplinares y la investigación interdisciplinar publicada en una gran variedad de revistas, que desafían los límites disciplinarios (Sjögårde & Ahlgren, 2018; Zhao, 2009). En tales casos, el conjunto de documentos recuperados contiene un ruido



considerable que afecta tanto a la precisión como a la exhaustividad. Para compensar estas limitaciones, se puede utilizar un método alternativo asignando a las categorías no solo revistas, sino también publicaciones (Glänzel & Schubert, 2003). De este modo, los sistemas de clasificación a nivel de publicaciones, como el que utiliza el CWTS (Traag et al., 2019; Waltman & van Eck, 2012) u otros propuestos en la literatura (Sjögårde & Ahlgren, 2020, 2018), pueden facilitar la delimitación. Sin embargo, el nivel de detalle de este tipo de clasificaciones puede ir en detrimento de las mismas, pues, en ocasiones, genera clasificaciones con un número muy reducido de artículos, dando lugar a clasificaciones demasiado extensas (Šubelj et al., 2016).

Tradicionalmente, han sido dos las bases de datos bibliográficas usadas para la delimitación de dominios científico: Scopus y Web of Science. En ambas bases de datos, la clasificación se realiza atendiendo al contenido de cada título de revista, a sus palabras clave y a los patrones de citación, pudiendo ser asignada una revista a una o varias categorías temáticas. Es decir, se asignan las revistas científicas a categorías teniendo en cuenta el alcance de la revista, así como el análisis de las citas de la revista. El sistema de clasificación basado en la asignación de revistas a categorías temáticas en WoS fue propuesto por Pudovkin y Garfield (2002). Este sistema se organiza en tres niveles. Un primer nivel que se estructura en 5 categorías generales, un segundo nivel con 153 áreas de investigación y un tercer nivel con 254 categorías temáticas (Clarivate, 2020). El sistema de clasificación utilizado en Scopus, denominado All Science Journal Classification (ASJC) (Franceschini et al., 2016; Wang & Waltman, 2016), se estructura en tres niveles. Un nivel superior que consta de 4 grandes áreas del conocimiento, un nivel intermedio con 27 áreas temáticas y un nivel inferior compuesto por 334 categorías temáticas (Elsevier B.V., 2020).

Por otro lado, el análisis de *clustering* es un método eficaz para ser utilizado en la delimitación de una amplia variedad de dominios científicos, tanto a

nivel de revistas como a nivel de publicaciones (Leydesdorff et al., 2017; Gómez-Núñez et al., 2016; Gómez-Núñez, Vargas-Quesada, & de Moya-Anegón, 2016; Wang & Waltman, 2016; Small et al., 2014; Gómez-Núñez et al., 2014, 2011; Zitt & Bassecouard, 2006). Además, los métodos híbridos, que combinan diferentes tipos de redes bibliométricas para estudiar las relaciones de las citas, son capaces de generar clústeres precisos (Glänzel & Thijs, 2017; Boyack & Klavans, 2014, 2010) en nuevas clasificaciones temáticas.

La combinación de los modelos para delimitar campos del conocimiento genera ventajas en el proceso de delimitación. Los sistemas de clasificación no captan de manera idónea el carácter multidisciplinar de algunas disciplinas ni cómo evolucionan, por lo que necesitan ser revisados periódicamente. No obstante, las técnicas de mapeo y *clustering* sí permiten la detección del carácter multidisciplinario de la ciencia y sus dinámicas de cambio, además de identificar subdominios científicos a través de redes bibliométricas o mapas de conocimiento. De igual modo, el uso de búsquedas para la recuperación de información complementa los sistemas de clasificación establecidos y permite ampliar las técnicas de mapeo y *clustering*, profundizando en cuestiones analíticas, por ejemplo, teorías o métodos utilizados en una disciplina, con el uso de publicaciones como unidades de análisis (Zitt et al., 2019).

La combinación de métodos en la delimitación temática ha sido estudiada a partir de búsquedas para la recuperación de información junto al análisis de citas, lo que permite ampliar un conjunto de datos recuperado inicialmente. Sin embargo, este método híbrido se vuelve problemático cuando, por ejemplo, el uso de términos comunes tiene una influencia negativa en la precisión, pero positiva en la exhaustividad. La recuperación total también puede verse afectada porque, a veces, los límites de los campos son difíciles de definir; y la ayuda de expertos en el campo para diseñar estrategias de

búsqueda puede producir un sesgo de especialización, lo que lleva a una visión general sesgada y superficial del dominio científico (Zitt, 2015).

Las técnicas de mapeo y *clustering*, junto con las redes de citación, también han sido usadas en los sistemas de clasificación. Vargas-Quesada (2005) propuso una metodología basada en la cocitación de revistas para representar la estructura científica de los dominios temáticos a nivel de categorías temáticas. Waltman & van Eck (2012) diseñaron un sistema de clasificación de publicaciones, basado en relaciones de citas directas entre las publicaciones indexadas en WoS, agrupándolas en áreas de investigación organizadas según una estructura jerárquica de tres niveles. Este tipo de delimitación a nivel de publicación coincide con mayor precisión con la estructura actual de la investigación científica de un campo científico. En consecuencia, el sistema de clasificación de publicaciones podría ayudar a definir un sistema a nivel de revista, pero podría resultar problemático si se hiciese, al contrario (Sjögårde & Ahlgren, 2020; Šubelj et al., 2016). Por tanto, la delimitación de dominios científicos a nivel de publicación es una posible solución cuando hay que enfrentarse a las limitaciones que implica la clasificación a nivel de revista (Perianes-Rodríguez & Ruiz-Castillo, 2017).

En la misma línea, Klavans y Boyack (2017) introdujeron un sistema de clasificación bastante detallado, con alrededor de 100.000 temas, usando las publicaciones indexadas en Scopus. Para ello, se dividen las publicaciones por temáticas mediante la agrupación de enlaces de citas directas. A continuación, se aplica una medida para clasificar la prominencia del tema con la finalidad de identificar aquellos que revelan la oferta y la demanda en los sistemas científicos. La delimitación de campos a este nivel temático ofrece la ventaja de predecir si un tema crecerá o descenderá, así como su contribución a la dinámica de la ciencia, en términos de la financiación recibida.

Investigaciones recientes han comparado diferentes sistemas de clasificación de revistas y publicaciones (Shu et al., 2019). Estos autores afirman la necesidad de desarrollar sistemas de clasificación de revistas y publicaciones robustos y precisos. Un aumento en el número de temas incluidos en un sistema de clasificación de revistas y de publicaciones tiene un efecto en la precisión y puede reducir la clasificación errónea de artículos. El mismo efecto se produce en un sistema de clasificación de revistas cuando incluye disciplinas amplias o de un alto nivel jerárquico, en lugar de muchas disciplinas (Gómez Núñez, 2016; Gómez-Núñez, Vargas-Quesada, Chinchilla-Rodríguez, et al., 2016; Gómez-Núñez, Vargas-Quesada, & de Moya-Anegón, 2016).

### **2.1.3. Estrategias de búsqueda**

El uso de estrategias de búsqueda para la recuperación de información de un dominio científico se considera el arquetipo de recuperación de información más comúnmente utilizado para la delimitación de campos del conocimiento. Las estrategias de búsqueda se definen como un conjunto de términos léxicos (palabras clave y sintagmas nominales) conectados con operadores booleanos (AND, OR y NOT) que nos permiten recuperar información (publicaciones científicas, patentes, etc.) (Maghrebi et al., 2011). La aplicación de estrategias de búsqueda complejas es ampliamente utilizada para recopilar el conjunto de documentos relacionados con un dominio científico. Sobre todo, este tipo de estrategias resultan fructíferas cuando hay que recuperar información de campos emergentes e interdisciplinarios, ya que cubre la mayoría de los aspectos del campo de manera efectiva (Glänzel, 2015).

Esta aproximación ha sido utilizada en diferentes bases de datos (WoS, Scopus, WIPO, USPTO, EPO, etc.). Concretamente, las estrategias de búsqueda por términos han permitido recuperar el conjunto de datos relevante para delimitar el dominio científico NST. Por ejemplo, se utilizó la raíz “nano” para recopilar todas las publicaciones que incluyan esta raíz en el

título (Dunn & Whatmore, 2002; Meyer et al., 2001; Tolles, 2001). Entre las primeras investigaciones que propusieron estrategias de búsqueda para estudiar la NST destaca la propuesta de Braun y sus colaboradores (1997). Estos autores utilizaron el prefijo “nano” para recuperar la producción científica, con el fin de analizar el crecimiento de las publicaciones del dominio temático. Esta misma estrategia fue empleada para dar respuesta, por ejemplo, al carácter multi o interdisciplinar de la NST y establecer sus patrones de colaboración (Schummer, 2004; Meyer & Persson, 1998); para estudiar la procedencia nacional de las revistas de NST y la identidad nacional de sus miembros editoriales, entre las que destacaron Estados Unidos, países asiáticos como China, Japón e India y, en menor medida, países de la Unión Europea como Reino Unido, Alemania y Francia (Braun et al., 2007). De nuevo, la investigación de revistas con prefijo “nano” reveló la pertenencia disciplinar, evidenciando que las revistas emergentes de NST provenían de campos como la nanobiología, la nanomedicina, la nanobiomedicina y la nanobiotecnología, mientras que la mayor parte de la producción científica en NST se publicaba en revistas de física, química y ciencia de los materiales (Andrievski & Klyuchareva, 2011).

Por otro lado, se combinó el prefijo “nano” con palabras clave de NST, excluyendo aquellos términos que contienen el prefijo “nano”, pero que nada tienen que ver con NST (Grieneisen & Zhang, 2011; Porter et al., 2008; Mogoutov & Kahane, 2007; Glänzel et al., 2003; Noyons et al., 2003). Por ejemplo, se analizaron los países más productivos y con mayor impacto, y su estructura temática (Youtie et al., 2008; Kostoff et al., 2007b; Kostoff, Koytcheff, et al., 2006; Kostoff, Murday, et al., 2006).

A pesar de todo, estas estrategias de búsqueda presentan inconvenientes. La basada únicamente en el prefijo “nano” excluye aquellas publicaciones que no contienen dicho prefijo y que pueden ser relevantes, como es el caso de los términos fullereno y grafeno. Por tanto, no proporcionan una delimitación sólida porque solo se cubre una pequeña parte del corpus temático de NST.

El hándicap de la estrategia de búsqueda basada en la combinación de estrategias de búsqueda es el sesgo a la especialidad. En estos casos, las consultas suelen estar respaldadas por la opinión de los expertos para incluir o excluir palabras clave. Además, la mayoría de las estrategias de búsqueda de NST han sido diseñadas teniendo en cuenta la sugerida por Glänzel et al. (2003), lo que provoca que los resultados obtenidos en términos de principales áreas temáticas y revistas en NST sean similares (Huang et al., 2011).

Varias han sido las investigaciones enfocadas a la mejora de las estrategias de búsqueda para el análisis de la NST (Arora et al., 2014, 2013; Maghrebi et al., 2011; Porter et al., 2008; Mogoutov & Kahane, 2007; Zucker et al., 2007). En ellas se ha estudiado la relevancia de ciertos términos y se han incluido nuevos términos, extraídos de las publicaciones de NST, atendiendo a los niveles de precisión y exhaustividad.

Otra de las mejoras llevadas a cabo fue la propuesta por Zitt y Bassecoulard (2006), que combinaron estrategias de búsqueda y análisis de citas para su delimitación. Esta combinación de modelos resultó altamente efectiva, debido a que aumenta la precisión y la exhaustividad en la recuperación de información, reduciendo considerablemente el ruido documental. En la misma línea, Leydesdorff y Zhou (2007) fusionaron la búsqueda con prefijo “nano” y técnicas de visualización basadas en análisis de citas y títulos de revistas.

La actualización y mejora de la estrategia de búsqueda realizada por Wang et al. (2019) reportó que el dinamismo de la NST obliga a revisar constantemente su terminología para realizar análisis precisos del campo y detectar términos emergentes de la investigación en NST. Estos autores sugirieron un procedimiento para recopilar un conjunto de datos que combinaba documentos recuperados por estrategias de búsqueda y documentos recuperados a través de la categoría temática de *Nanoscience &*

*Nanotechnology* de la WoS. Los resultados evidenciaron que muchas de las investigaciones en NST no están cubiertas por la categoría temática de WoS.

#### **2.1.4. Análisis de dominios científicos**

Desde que Thomas Kuhn (1962) expusiese su concepto de revolución científica, los estudios sobre dominios científicos se han basado en las interacciones y comportamientos del conocimiento (Held et al., 2021). Kuhn determinó tres fases en el proceso de evolución científica: ciencia normal, crisis y revolución. Según esta teoría, la evolución de la ciencia no progresa de manera uniforme, sino que existe un momento en la ciencia normal durante el cual se genera un nuevo paradigma (el conjunto de teorías, métodos y consenso de la comunidad científica, con la finalidad de dar soluciones a los problemas existentes), ya que el existente no es capaz de explicar todo lo que se conoce. De tal manera que para que exista un cambio de paradigma (o revolución) debe haber una crisis del existente.

Atendiendo a todos estos elementos, el análisis de dominios científicos es el paradigma metodológico utilizado para examinar la ciencia desde diversas dimensiones. Este implica la observación de la actividad de la comunidad científica vinculada a una disciplina o especialidad científica. Dentro de un dominio científico se establece una organización de conocimiento, una estructura y unos patrones de colaboración y de comunicación (por ejemplo, las revistas científicas) que permiten transmitir el conocimiento a los miembros de la comunidad científica a través de un lenguaje o vocabulario especializado, lo que posibilita conocer el dominio científico desde una perspectiva holística (Hjørland & Albrechtsen, 1995).

Shneider (2009) apuntaba a que el proceso de evolución científica se puede dividir en cuatro fases. La primera fase consiste en establecer los objetivos de la investigación dentro de un dominio científico, para dar respuesta a nuevas preguntas. En la segunda fase aparecen los instrumentos científicos para que los investigadores puedan desarrollar su trabajo. La tercera fase

consiste en desarrollar la investigación, aplicando los nuevos métodos y técnicas para poder responder a las preguntas de investigación. La última fase continúa con el desarrollo del conocimiento generado y su transferencia a la comunidad científica a través de los canales de comunicación científica. De este modo, sería en la fase 3 de la evolución de una disciplina científica cuando pueden aparecer nuevas líneas de investigación o dominios científicos emergentes.

Sin embargo, son varias las dimensiones desde las que se puede abordar el estudio de la ciencia, no solo desde la dimensión científica, sino también desde lo social, político o económico. Por tanto, si debemos atender a las distintas dimensiones para estudiar un dominio científico, debemos tener en cuenta diferentes metodologías. Hjørland (2002) propuso once métodos para llevar a cabo el análisis de dominios científicos, entre los que se encuentran los estudios bibliométricos. Destaca de ellos la solidez para el análisis de dominios científicos, pues son empíricos y proporcionan información muy detallada sobre las conexiones entre documentos. Igualmente, la bibliometría permite la combinación de distintos métodos como el análisis de redes de citación (Karunan et al., 2017; Glänzel, 2012; McCain et al., 2005) y la visualización de información (Carley et al., 2017; Wen et al., 2017; Börner et al., 2005), los cuales resaltan las características de los dominios científicos, proporcionando una visión enriquecedora de los mismos.

Así, profundizar en el dinamismo de la epistemología desde una perspectiva bibliométrica permite identificar paradigmas emergentes en los diversos campos del conocimiento (Chen, 2017). En el caso de los dominios científicos interdisciplinarios, el análisis de dominios científicos debe incorporar métodos que faciliten el estudio de las peculiaridades de este tipo de dominios, como son la integración del conocimiento entre las diferentes disciplinas, actores, problemas de investigación, etc. (López-Huertas, 2015).



### **2.1.5. Análisis de citas**

La cita permite rastrear el flujo de ideas y conocimiento, ya que los autores citan cuando arraigan o apoyan sus ideas en documentos publicados, estableciendo así un nexo entre documentos (Garfield & Merton, 1979; Narin, 1976). En los procesos de comunicación de la ciencia, la mención a una publicación es un medio de manifestar la relación entre el trabajo citante y el trabajo citado en un punto particular del desarrollo de la investigación (Egghe & Rousseau, 1990; Sandison, 1989).

El análisis de citas ha sido y es uno de los métodos más utilizados en los estudios cuantitativos de la literatura científica y tecnológica (MacRoberts & MacRoberts, 1996) para evaluar la calidad de la investigación (Small, 1978). Aunque los resultados deben ser interpretados atendiendo no solo a los aspectos intelectuales, sino a los sociológicos (Aksnes et al., 2019). No obstante, el análisis de citas ha demostrado un gran poder de predicción del impacto de la producción científica (Abramo et al., 2019), lo que facilita detectar la investigación emergente y destinar recursos hacia esas oportunidades detectadas. La importancia e interés de este enfoque se ven reflejados en la constante mejora y refinamiento del recuento de la citas en los últimos años (Bornmann et al., 2020; Small et al., 2019).

Entre las propuestas basadas en el análisis de citas para delimitar la estructura de la ciencia y la tecnología encontramos: citación directa, cocitación y emparejamiento bibliográfico. El análisis de citación directa ha sido esencial para el rastreo de conceptos emergentes, el desarrollo histórico de los avances de los dominios científicos y la delimitación de frentes de investigación y categorías temáticas. En los últimos años, la citación directa ha revelado los mejores resultados a la hora de delimitar el conocimiento, tanto el científico como el tecnológico, pues permite realizar agrupaciones más precisas que cuando se utiliza el análisis de cocitación o el emparejamiento bibliográfico (Klavans & Boyack, 2017a). De igual modo, el

emparejamiento bibliográfico ha permitido determinar publicaciones recientes y frentes de investigación, aunque mostrando deficiencias en la identificación de publicaciones no tan recientes (Boyack & Klavans, 2010). El análisis de cocitación se considera eficaz en la delimitación e identificación de frentes de investigación (Small et al., 2014), pese a que resulta menos preciso que el análisis de citación directa o el emparejamiento bibliográfico (Waltman et al., 2020).

Por otra parte, la excelencia en la investigación ha sido un mantra en las agendas científicas de los países y el análisis de citación se ha usado como herramienta de apoyo en estos procesos (Danell, 2011). Por ejemplo, se han usado los artículos altamente citados en el desarrollo de sistemas de información científica que faciliten caracterizar y clasificar diferentes unidades de análisis (Bornmann, 2014).

Las publicaciones altamente citadas (*Highly Cited Papers*) determinan dinámicas científicas interesantes al permitir conocer hallazgos, contribuciones, enfoques, métodos de investigación y desafíos de un dominio científico (Van Noorden et al., 2014; Glänzel & Schubert, 1992). Tienen la capacidad de apuntar a temas en los que la comunidad científica estaba o sigue activa e identificar a los investigadores más citados para, por ejemplo, establecer futuras colaboraciones (Aksnes, 2003). También han servido para estimar la tasa de crecimiento per cápita y la calidad de las publicaciones por regiones dentro del desarrollo de la NST (Zhu et al., 2017) o para caracterizar las dinámicas de citación en NST en la década de los 90 (Rogers, 2010).

Además, las publicaciones altamente citadas son consideradas las publicaciones influyentes (*Seminal Papers*). Estas publicaciones no solamente tienen un gran impacto en la comunidad científica de un dominio científico específico, revelando a los investigadores con más peso dentro del mismo, sino que muestran las implicaciones sociales y políticas que rodean un área emergente de la ciencia (Small et al., 2008). El desarrollo histórico de los

avances de la NST ha sido estudiado en diversos trabajos, a partir de los *seminal papers*, para analizar el desarrollo intelectual del dominio científico NST (Aleixandre-Tudó et al., 2020; Kostoff, Murday, et al., 2006; Kostoff, Stump, et al., 2006; Kostoff & Shlesinger, 2005).

#### **2.1.6. Investigación multidisciplinar, interdisciplinar y transdisciplinar**

Estudios previos han analizado si la NST se caracteriza por ser multidisciplinar, interdisciplinar y transdisciplinar. Estos tres adjetivos han servido para singularizar los dominios científicos, aunque existe cierta confusión sobre el uso de estos términos.

El adjetivo *multidisciplinar* suele asignarse a dominios científicos que muestran relaciones con otros campos del conocimiento, pero donde no se logra integración; *interdisciplinar* se designa a dominios científicos que establecen fuertes vínculos, superposición o integración con otros campos del conocimiento, dando lugar a una identidad teórica, conceptual y metodológica; mientras que *transdisciplinar* se atribuye a la investigación que presenta convergencia entre dominios científicos, acompañada de una integración mutua (Morillo et al., 2003).

Sin embargo, es difícil asignar este tipo de adjetivos, como es el caso de interdisciplinar, si los dominios no han sido previamente bien definidos (Krishnan, 2009). En esta misma línea, dependiendo de la situación en la que se usa un término tan polifacético, interdisciplinar puede tener diferentes significados (Leydesdorff & Rafols, 2011; Porter & Rafols, 2009). Por consiguiente, la compleja y generalizada definición de interdisciplinaridad convierte su asignación en un proceso discutible (Sugimoto & Weingart, 2015).

Los primeros autores que investigaron la interdisciplinaridad de la NST revelaron que las revistas de física, seguidas de las revistas multidisciplinarias, son las que publicaban el mayor número de artículos de

NST (Meyer & Persson, 1998). El estudio de Schummer (2004), a través del análisis de coautores, argumentó que la mayor parte de las revistas en nanotecnología recibían artículos de investigadores con una sola afiliación disciplinar, escritos en su mayoría por físicos. Además, el ritmo de participación de científicos e ingenieros de diversas disciplinas, países e instituciones en la investigación a nanoescala era notable. El desarrollo de la investigación de esta disciplina científica debería acompañarse de nuevas formas y grados de multi e interdisciplinariedad, así como de la colaboración institucional y geográfica. Esto no sucede, ya que no existen patrones particulares ni grados de multi ni interdisciplinariedad fijos, pues depende de los diferentes campos de investigación disciplinarios que se relacionan entre sí y que no comparten mucho más que el prefijo “nano” (Schummer, 2004). Asimismo, Rafols y Meyer (2007) corroboraron que existe un alto grado de interdisciplinariedad en la dimensión cognitiva (estructura del conocimiento) de la NST, pero que ese grado de interdisciplinariedad disminuye en la dimensión social (comunidad científica).

Bassecoulard, Lelu y Zitt (2007) analizaron la estructura multidisciplinar o interdisciplinar de la NST. En su estudio realizaron una clasificación de publicaciones en clústeres temáticos conectados por la similitud de sus referencias y técnicas de emparejamiento bibliográfico. Evidenciaron el moderado nivel multidisciplinar del dominio científico, debido a que la mayoría de las temáticas estaban relacionadas con física y química. Pero la estructura a nivel micro –referencias de las publicaciones de NST– sí mostraba una verdadera interdisciplinariedad, lo que podía significar la convergencia de dominios científicos.

No obstante, esta interdisciplinariedad fue bien definida como convergencia NBIC (Nano-Bio-Info-Cogno) = (Nanotechnology, Biotechnology, Information Technology and Cognitive Science) (Roco & Bainbridge, 2002), que combina los avances de cuatro amplios campos científico-técnicos poco relacionados entre sí y con distinto grado de consolidación. Dicha convergencia no se basa

solamente en la parte teórica de las ciencias, sino que contempla también la parte tecnológica. Como consecuencia, se designa la convergencia como una de las principales características de la NST, pues exhibe un alto grado de diversidad de disciplinas que enfocan su investigación a nanoescala, definiendo a la nanotecnología como “una colección de campos multidisciplinares” que son capaces de integrar sus conocimientos en NST de diferentes maneras (Porter & Youtie, 2009b).

El carácter multidisciplinar de la NST también se reflejó durante las primeras etapas de su desarrollo, cuando se lograron los avances conceptuales y tecnológicos. La publicación de los artículos de NST se realizaba en una amplia variedad de revistas y la terminología dominante presente en esas publicaciones determinó conexiones predominantemente con física, química, ciencia de los materiales y biociencias (Milojević, 2012).

Estudios recientes alegan que existe un mayor grado de interdisciplinaridad durante los primeros años, pero disminuye ligeramente con el paso del tiempo (Finardi & Lamberti, 2021). No todos los dominios científicos que nutren los conocimientos de NST (física, química, biología, etc.) aportan de igual manera y, en la actualidad, ciencia de los materiales es el campo de conocimiento que más contribuye en NST.

### **2.1.7. Visualización de información**

Visualizar la información ayuda a hacer más comprensible la organización de conocimiento, además de revelar patrones y tendencias que subyacen de los datos, como, por ejemplo, las características, estructura y dinámicas de un campo de conocimiento a través de su literatura científica (Zhao & Strotmann, 2015; Vargas-Quesada et al., 2010).

En los estudios cuantitativos de ciencia y tecnología, las técnicas de visualización de información se han utilizado para el mapeo de dominios científicos en 2D y 3D. Dichas técnicas han sido muy útiles para la

recuperación de información y la clasificación (Gómez-Núñez et al., 2016; Vargas-Quesada & de Moya-Anegón, 2007). Sin embargo, en la visualización de dominios científicos debemos tener en cuenta cuestiones como la fuente de datos a elegir, cómo se van a analizar y visualizar esos datos y cómo se va a dar sentido a lo que se nos muestra en la imagen.

Sobre todo, la visualización de dominios científicos se basa en la representación espacial, mostrando las interrelaciones entre los diferentes subdominios. Para una correcta visualización, Börner et al. (2005) sugieren la siguiente secuencia de pasos a tener en cuenta: 1) extracción de datos; 2) unidad de análisis; 3) selección de métricas; 4) cálculo de la similitud entre las unidades de análisis; 5) asignación de coordenadas a las unidades de análisis; y 6) análisis e interpretación de la visualización.

El estudio de diferentes unidades de análisis permite examinar los diversos aspectos de un dominio científico. Las unidades de análisis más usadas en la visualización de campos del conocimiento han sido revistas, publicaciones, autores y términos (Boyack et al., 2005; Ding et al., 2000; He, 1999; White & McCain, 1998). No obstante, también se han llevado a cabo visualizaciones de grandes dominios científicos, utilizando las categorías temáticas como unidad de análisis (Vargas-Quesada et al., 2010, 2008).

Dentro de la visualización de la información se enmarcan los mapas de la ciencia. Se trata de representaciones gráficas de la estructura de la investigación científica en dominios temáticos. Permiten explorar las relaciones entre los distintos elementos (publicaciones, instituciones, países, áreas temáticas, etc.), a la vez que dan información de la evolución intelectual, cognitiva y social (Chen et al., 2015; Vargas-Quesada et al., 2010, 2008; Moya-Anegón et al., 2007; Vargas-Quesada & de Moya-Anegón, 2007; Noyons, 2001). En otras palabras, revelan aspectos estructurales y dinámicos de la investigación científica, lo que los convierte en instrumentos de gran utilidad en el diseño de agendas científicas.

Los mapas de la ciencia pueden generarse a nivel global y a nivel local. Sin embargo, cuando se llevan a cabo comparativas, los mapas a nivel local son problemáticos debido a que las posiciones de las unidades representadas ofrecen inestabilidad. Con objeto de solventar esta problemática, existe la opción de generar un mapa global del que tomar como referencia las posiciones de las unidades representadas para, a continuación, superponer sobre él la información que se quiere visualizar y analizar (Rafols et al., 2010). Esta definición atiende al concepto de mapas solapados. Los mapas solapados son considerados una herramienta muy poderosa para explorar ciertos comportamientos de la ciencia y estudiar las dinámicas, cada vez más fluidas y complejas, de la misma (Carley et al., 2017; Vargas-Quesada et al., 2017; Leydesdorff et al., 2013).

Las primeras visualizaciones en cienciometría se cimentaron en el análisis de citas, donde se representaba la estructura intelectual de un campo (histograma) (Garfield et al., 1964). Años más tarde, apareció el concepto de mapas longitudinales que mejoraron los histogramas (Garfield, 1994), permitiendo detectar los trabajos más importantes de un campo científico y predecir los posibles avances científicos del mismo. Recientemente, y apoyándose en esta misma idea, se han desarrollado herramientas para la visualización, como el caso de CitNetExplorer (van Eck & Waltman, 2017, 2014), VOSviewer (van Eck & Waltman, 2010) o CiteSpace (Chen, 2006, 2004). Para una revisión más completa de estas herramientas, remitimos a Moral-Muñoz et al. (2020).

Con respecto a las técnicas, el análisis de cocitación y copalabras son métodos utilizados para visualizar distintas dimensiones de campos de conocimiento, estableciendo conexiones entre citas, autores, revistas o términos (Moya-Anegón et al., 2004). La medida de similitud entre las unidades de análisis que se usen para establecer las relaciones puede calcularse teniendo en cuenta los vínculos de citación o la coocurrencia,

(palabras, autores, países, etc.), permitiendo agrupar conceptos relacionados entre sí.

Aunque hay muchos análisis posibles para visualizar dominios científicos (Panta et al., 2016), como, por ejemplo, el uso de las denominadas altmétricas (García-Villar, 2021) o el estudio de las patentes (Jürgens, 2016), entre otros, esta tesis se centra en la revisión de mapas de la ciencia a partir de los datos bibliográficos contenidos en la producción científica.

#### **2.1.7.1. Análisis de copalabras**

La predicción es la esencia de la ciencia. Las palabras que confluyen en un dominio científico nos llevan a familiarizarnos con las ciencias vivas y tienen la capacidad de reflejar contenidos científicos, sociales y políticos que pertenecen a los dominios temáticos más controvertidos o áreas emergentes menos entendidas. Luego las palabras pueden también tener la capacidad de ayudar a predecir ciertas dinámicas científicas (Callon et al., 1991, 1983).

Cuando se estudia la producción científica de un campo del conocimiento, la similitud que muestran dos publicaciones puede medirse en función del número de palabras coincidentes entre ambas. Por consiguiente, a mayor coincidencia de palabras, más probabilidad de pertenecer a un mismo dominio o subdominio científico (Noyons et al., 1999; Noyons & Van Raan, 1998).

El análisis de copalabras es el arquetipo utilizado para estudiar la asociación entre los términos más representativos de la literatura científica, (Li & Chu, 2017; Cantos-Mateos et al., 2014, 2012; Ding et al., 2001; Coulter et al., 1998). Estos análisis ayudan a describir, definir e identificar los temas de investigación dentro de un dominio científico, así como a predecir futuras tendencias en la investigación (Callon et al., 1991). Reúnen términos contenidos en las publicaciones, extraídos normalmente de las palabras clave, título, resumen (Leydesdorff & Welbers, 2011) o texto completo (van



Eck et al., 2010), con los que se construye una matriz de proximidad/similitud, para capturar los cambios de un dominio científico a lo largo del tiempo. Mediante el estudio de la terminología correspondiente a diferentes períodos, el análisis de copalabras dibuja una imagen de las estructuras cognitivas y las dinámicas de desarrollo de los dominios científicos. Del mismo modo, proporciona información sobre los principales temas de investigación que los integran o sobre los que prevalecen en un período de tiempo determinado (Chen & Xiao, 2016; Börner et al., 2005; Braam et al., 1991a, 1991b).

La representación gráfica de una red de copalabras se ejecuta de dos maneras. Combinando las frecuencias de aparición de términos con las técnicas de representación espacial, fundamentadas en el escalado multidimensional (MDS) o combinando esas frecuencias con el análisis de redes.

La similitud de copalabras se fundamenta en el número de veces que dos palabras aparecen conjuntamente. En este contexto, en el Modelo de Espacio Vectorial (Salton et al., 1975) cada documento se representa como un vector. A cada término se le asigna un peso dentro del documento que determina la importancia de ese término. La similitud entre dos documentos se establece por la distancia entre los vectores, calculada gracias a los coeficientes de similitud. Esto permite su organización en grupos más pequeños, siendo los documentos de un mismo grupo más similares entre sí que los del resto de grupos.

También se ha usado el análisis de clúster (*cluster analysis*) como método estadístico multivariante que clasifica grandes cantidades de información en grupos manejables y significativos, siendo muy homogéneas las unidades de un mismo grupo y heterogéneas con respecto al resto de grupos (Waltman et al., 2020; Gómez Núñez, 2016; Gómez-Núñez, Vargas-Quesada, & de Moya-Anegón, 2016; Gómez-Núñez et al., 2014; Chen, 2013).

El análisis de copalabras se popularizó en la década de los 80 (Leydesdorff, 1989; Callon et al., 1983) y se ha ido perfilando con posterioridad (Leydesdorff & Nerghes, 2017) como un método eficaz para conocer y explicar la estructura cognitiva de un campo a nivel de especialidades de investigación (Braam et al., 1991a, 1991b; Small & Griffith, 1974), así como para revelar nuevos desarrollos de un dominio científico a lo largo del tiempo (Vargas-Quesada et al., 2017; Peters & van Raan, 1993). Este tipo de análisis se aplicó a la química de polímeros (Callon et al., 1991), a la investigación de redes neuronales (Van Raan & Tijssen, 1993), a la recuperación de información (Ding et al., 2001), a las ciencias de la información (van den Besselaar & Heimeriks, 2006), a la responsabilidad social empresarial (Qin et al., 2016) o a la COVID-19 (Colavizza et al., 2021) entre otros.

Aplicado al dominio científico NST, el análisis de copalabras ha cumplido diferentes propósitos. Por un lado, ha permitido detectar nanotecnologías de próxima generación, especialmente en el campo de la nanobiotecnología y la ingeniería de nanomateriales (Suominen et al., 2016). Por otro, ha determinado los frentes de investigación en algunas áreas como, por ejemplo, nanomedicina, concretamente en la terapia contra el cáncer (Li & Chu, 2017) o en áreas como el medio ambiente, la salud y la seguridad (Radhakrishnan et al., 2017).

#### **2.1.8. Especialización temática y ventaja competitiva**

Dentro de los estudios de ciencia y tecnología, la ventaja competitiva es una noción que permite medir la producción científica de un país en una temática determinada respecto a la producción global (Hidalgo et al., 2007). Las economías de los países crecen cuando se mejoran los productos y servicios que generan, pero, para ello, es imprescindible conocer qué se puede mejorar. De este modo, los países pueden ser más competitivos cuando se fomentan o explotan determinados productos que, aunque representen un

cambio en las estructuras de producción de mayor envergadura, garantizan su crecimiento.

El rendimiento científico realizado por los países en un determinado dominio científico, a nivel global, desvela las relaciones dentro de la estructura competitiva de dicho dominio. Que los países puedan centrarse en temas novedosos de un campo del conocimiento, aprovechando las fortalezas que presentan, les facilita la especialización y la diversificación a través de actividades relacionadas, dando lugar al desarrollo futuro de los territorios y generando activos en ellos (Foray, 2014).

El marcado carácter multidisciplinar de la NST podría conducir a la especialización en ciertos temas de investigación por parte de determinados territorios, los cuales se manifiestan a través de patrones específicos de especialización. Conocer los patrones de especialización a nivel de país o institución tiene implicaciones políticas, ya que ayuda a identificar la ventaja relativa con respecto a los colaboradores o competidores a nivel mundial y revela las fortalezas y debilidades nacionales dentro de los dominios científicos para, en consecuencia, establecer prioridades (Rousseau, 2019, 2018; Rousseau & Yang, 2012; Zhang et al., 2011; Glänzel, 2000). Promover esfuerzos de transformación y ganar una mayor ventaja competitiva, especialmente cuando los recursos económicos destinados a la ciencia son escasos, ayuda en el desarrollo de políticas para poder seleccionar y priorizar áreas donde se pueden desarrollar las actividades innovadoras con una ventaja competitiva de alto valor. Esto es lo que se conoce como Smart Specialisation o Especialización Inteligente (European Commission et al., 2021; OECD, 2013; Foray et al., 2009).

Descubrir a los agentes involucrados activamente que presentan un mayor potencial para futuras especializaciones minimiza los riesgos a la hora de establecer prioridades de investigación y puede beneficiar en los procesos de diseño y desarrollo de los sistemas nacionales de innovación. La posibilidad

de dotar a estos sistemas con herramientas, que les permitan identificar y priorizar la actividad de la investigación de un área emergente, puede ser de gran utilidad para vincular especialización y competitividad en el establecimiento de políticas selectivas y estructuras de incentivos a favor del desarrollo económico y bienestar social. De hecho, el desarrollo de estrategias de especialización inteligente manifiesta una gran capacidad de transformación en los territorios menos avanzados (Balland et al., 2019; McCann & Ortega-Argilés, 2015).

Otra noción clave es la capacidad de absorción de conocimiento, entendida como el conjunto de procesos para adquirir, asimilar, transformar y explotar el conocimiento con el fin de generar dinámicas más eficientes (Zahra & George, 2002; Cohen & Levinthal, 1990). Cuando se transfiere el conocimiento, saber aprovecharlo, para su posterior transformación en productos o servicios, es esencial en el desarrollo de procesos de transferencia tecnológica que mejoren realmente la eficacia de las entidades (Heinzl et al., 2013).

El vínculo entre los tres elementos —especialización temática, ventaja competitiva, absorción del conocimiento— determina la ventaja competitiva de los países respecto a sus competidores y cómo los competidores/colaboradores absorben conocimiento de los países especializados. De esta manera, la especialización temática adquiere mucha importancia en las otras *hélices* al ser un ente clave para que surjan oportunidades o se produzcan cambios que favorezcan al resto de elementos (Coveri & Zanfei, 2022; Fagerberg & Srholec, 2017a).

## **Capítulo 3. Justificación y objetivos**

### **3.1. Justificación de la tesis**

La delimitación de dominios científicos emergentes, especialmente aquellos con un marcado carácter multi/interdisciplinar, plantea dificultades. No todas las áreas de conocimiento presentan las mismas dinámicas de comportamiento o grados de intensidad en su desarrollo. De este modo, las temáticas que integran un dominio científico pueden estar muy consolidadas, en fase de desarrollo, emergiendo, fusionándose, desapareciendo, etc.

Todo ello provoca ciertas dificultades en el diseño y la elaboración de protocolos para la categorización de dominios científico en bases de datos. Categorizar el conocimiento es esencial para poder recuperarlo y, posteriormente, analizarlo. La delimitación de una categoría temática y su actualización necesitan ser abordadas desde distintos enfoques y usando distintas unidades de análisis (palabras clave, publicaciones, revistas, autores, niveles geográficos, etc.).

La categorización de los campos de conocimiento en las dos grandes bases de datos bibliográficas de carácter multidisciplinar, Scopus y WoS, permite el análisis de dominios científicos. Sin embargo, la falta de normalización entre los sistemas puede ir en detrimento de las comparativas y consistencia de los análisis bibliométricos.

Aunque la NST es ya un dominio científico claramente establecido, su elevado dinamismo y su carácter multidisciplinar sobrepasa las fronteras de las clasificaciones temáticas establecidas en las grandes bases de datos. La ausencia de una adecuada clasificación dificulta los procesos técnicos y analíticos a la hora de estudiarla. Hasta el momento, WoS es la única base de datos internacional y multidisciplinar, con similares prestaciones a Scopus, donde la categoría Nanociencia y Nanotecnología está delimitada desde el año 2005. Sin embargo, esta categoría temática no existe en la base de

datos Scopus, aunque contiene tanto revistas que recoge WoS en esta categoría como otras que no están contenidas en WoS y sí en Scopus. Esta ausencia de clasificación de la NST en Scopus limita la representatividad de la información recuperada a través de las categorías temáticas establecidas y limitadas a un conjunto de documentos. Por tanto, se pone de manifiesto la oportunidad/necesidad de estudiar su delimitación temática en la base de datos Scopus.

Mi Trabajo Fin de Máster fue el germen de esta tesis doctoral. Después de una exhaustiva revisión bibliográfica y basándonos en la producción científica de la categoría *Nanoscience & Nanotechnology* en Web of Science, pudimos examinar algunas características de la NST, como, por ejemplo, que los artículos más citados en NST no habían sido publicados en revistas especializadas en NST.

La omisión de revistas en la base de datos WoS pudo determinarse gracias a las primeras pruebas para la delimitación de NST en Scopus. En 2012, se elaboró y puso en práctica la primera estrategia de búsqueda, se desarrolló un método de identificación y se delimitó el conjunto de revistas de Nanociencia y Nanotecnología (Muñoz-Écija et al., 2013). La aplicación de los resultados obtenidos en estas primeras pruebas dio lugar al desarrollo y implementación de la categoría *Nanoscience and Nanotechnology*<sup>8</sup> en el portal bibliométrico Scimago Journal & Country Rank en el año 2015, donde se incluía el conjunto de revistas identificadas por la metodología desarrollada. Este trabajo también fue utilizado para crear la categoría *Sports Science*. Sin embargo, a pesar de que los resultados obtenidos pudieron ser aplicados, la delimitación propuesta no es suficiente y que hay que seguir investigando en esta línea.

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<sup>8</sup> <https://www.scimagojr.com/journalrank.php?category=2509&type=j>

Con el propósito de profundizar y refinar más en la delimitación de la NST, se presentó un proyecto de investigación<sup>9</sup> sobre el estudio de Nanociencia y Nanotecnología a nivel nacional e internacional en la convocatoria del Programa Estatal de Investigación, Desarrollo e Innovación Orientada a los Retos de la Sociedad, Convocatoria 2014, Modalidad 1: «Proyectos De I+D+I», Spain. (Ref. CSO2014-57770-R). Esta tesis se ha realizado en paralelo al desarrollo de este proyecto del plan nacional.

Por otro lado, la revisión de la literatura dejó patente que son diversas y necesarias las combinaciones de técnicas empleadas para la delimitación de dominios científicos. Por consiguiente, en esta tesis se aborda la problemática de identificación de categorías científicas, cuya metodología será transversal y aplicable a cualquier campo de investigación emergente.

En particular, la delimitación de la NST ayudará a la comunidad científica en la recuperación y acceso a la producción científica, en la adquisición de nuevos conocimientos y en la resolución de problemas relacionados con la investigación del dominio científico. Dada la importancia estratégica de los sistemas de investigación e innovación, una mejor comprensión de los avances en el campo de la NST puede beneficiar a los gestores de investigación.

### **3.2. Objetivos**

El objetivo general es estudiar la delimitación de campos científicos en bases de datos multidisciplinares o especializadas, a través de la aplicación de diferentes enfoques. Creemos que los resultados de esta tesis pueden ser útiles a los investigadores del área para conocer mejor la problemática de las clasificaciones y, también, para realizar diagnósticos de la estructura

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<sup>9</sup> Nanociencia y Nanotecnología: Análisis métrico del liderazgo nacional e internacional, excelencia científica, capacidad de transferencia al sector productivo y visibilidad web. Funded by: Programa Estatal de Investigación, Desarrollo e Innovación Orientada a los Retos de la Sociedad, Convocatoria 2014, Modalidad 1: «Proyectos De I+D+I», Spain. (Ref. CSO2014-57770-R), 2015 - 2017.

cognitiva e intelectual de la producción científica en combinación con indicadores de especialización temática. Para ello nos centramos en Nanociencia y Nanotecnología como estudio de caso y aplicamos esta delimitación a nivel de país.

Con la finalidad de lograr dicho objetivo se plantean los siguientes objetivos específicos:

1. Desarrollar un protocolo para la delimitación de la categoría temática NST en una base de datos de carácter multidisciplinar a partir de estudios previos.

1a. Identificar el corpus temático de NST con la selección de revistas semilla del *Journal Citation Reports* (JCR) de WoS.

1b. Agrupar las estrategias de búsqueda propuestas en la bibliografía especializada.

1c. Analizar la citación de las revistas semillas de WoS para determinar:

1c.1. Documentos clave de NST, autores y revistas dónde se han publicado y cuáles son sus patrones de citación;

1c.2. Revistas más citadas;

1c.3. Principales líneas de investigación en NST y su evolución.

1d. Identificar el corpus temático de NST, a partir de la agrupación y estrategias de búsqueda descritas en la bibliografía, y de las listas de revistas de la categoría *Nanoscience and Nanotechnology* en JCR y SJR.



1e. Seleccionar el conjunto de revistas nucleares que conformarán la categoría NST mediante la combinación de varias técnicas (Capítulo 4, Apartado 4.2.2).

2. Análisis de los frentes de investigación a partir del análisis de copalabras.

2a. Determinar los principales frentes de investigación en NST para comparar a España con otros países.

2b. Identificar la evolución de los frentes de investigación más punteros.

2c. Visualizar los frentes de investigación y su evolución a nivel mundial y nacional.

2d. Determinar la especialización de los países en cada uno de los frentes de investigación.

3. Identificar la especialización en función de la producción global usando el conjunto de documentos recuperados en los puntos 1 y 2.

3a. Estudiar la especialización por países.

3b. Analizar la especialización de los diferentes subcampos temáticos por países a nivel de publicación y a nivel de términos.

### **3.3. Preguntas de investigación**

Esta tesis trata de dar respuesta a las siguientes preguntas de investigación:

1. ¿Cuál es la estructura intelectual y cognitiva de la NST?

Partiendo de la premisa de que las referencias bibliográficas citadas en trabajos de investigación son un indicador de la influencia que tienen en la comunidad científica, condicionando el progreso científico

y dando lugar a nuevas ideas y áreas temáticas, se busca detectar el origen y trazar la evolución de la estructura intelectual del dominio científico objeto de estudio de esta tesis, la NST. Al mismo tiempo, la similitud entre las palabras contenidas en la literatura producida dentro de un dominio científico es otro indicador de la asociación entre las palabras más representativas de la literatura científica de dicho campo del conocimiento. Por tanto, el objetivo es identificar y analizar la estructura cognitiva a lo largo del tiempo, es decir, sus líneas o frentes de investigación, para mostrar los cambios que se están produciendo dentro del dominio científico.

2. ¿Cuáles son las cuestiones a tener en cuenta a la hora de la delimitación de dominios científicos emergentes?

Se explorarán y compararán diferentes metodologías utilizadas para la delimitación de dominios científicos atendiendo a las diferentes unidades de análisis. Los grados de precisión y exhaustividad se determinarán para cada una de las metodologías aplicadas a través de la consulta a expertos.

3. ¿Cómo podemos identificar y rastrear la competitividad, en términos de especialización, en las líneas de investigación de un dominio científico a nivel mundial y nacional?

Los patrones de especialización revelan la ventaja relativa con respecto a colaboradores o competidores a nivel mundial, permitiendo promover esfuerzos eficaces para la transformación de los países. Utilizando técnicas para explorar la estructura cognitiva y medir la especialización de la producción científica de NST en varios países, el objetivo es identificar y analizar los principales frentes de investigación, así como su ventaja competitiva en cada país con respecto al mundo.

## Capítulo 4. Material y métodos

En este capítulo se describen los aspectos metodológicos básicos de la investigación realizada en esta tesis doctoral. Todas las propuestas metodológicas que integran este capítulo son las presentadas en las publicaciones de la Parte II de esta tesis.

### 4.1. Fuente de datos

Las bases de datos bibliográficas mayormente utilizadas para la delimitación de campos científicos y la realización de estudios bibliométricos han sido Scopus y Web of Science. Actualmente, existen muchos más productos de este tipo, como por ejemplo Dimensions, OpenAlex, etc. Para una revisión del mercado de bases de datos con uso bibliométrico remitimos a Singh Chawla (2022); Martín-Martín et al. (2021); Visser et al. (2021); Huang et al. (2020).

WoS y Scopus son consideradas las fuentes de información de referencia en la evaluación de la investigación e incluyen indicadores relativamente fiables para estudios cuantitativos de la ciencia (Park et al., 2016). Aunque la cobertura de las revistas en Scopus es mayor y con menos sesgos geográficos y temáticos que en WoS (Gusenbauer, 2022; Mongeon & Paul-Hus, 2016; Leydesdorff et al., 2010; de Moya-Anegón et al., 2007).

Scopus<sup>10</sup> es una base de datos bibliográfica de carácter multidisciplinar lanzada en noviembre de 2004 por Elsevier. Con más de 75 millones de registros y unos 25.100 títulos, Scopus organiza su contenido en 4 grandes áreas del conocimiento (ciencias de la vida, ciencias físicas, ciencias de la salud y ciencias sociales y humanidades - life sciences, physical sciences, health sciences and social sciences & humanities) que se dividen en 27 áreas y 334 categorías temáticas.

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<sup>10</sup> <https://www.scopus.com>

WoS<sup>11</sup>, que actualmente pertenece a la empresa Clarivate Analytics, fue la primera y única gran base de datos bibliográfica de carácter multidisciplinar hasta la aparición de Scopus. Su colección está compuesta por 10 índices, entre los que destacan el Science Citation Index Expanded (SCI-EXPANDED), Social Sciences Citation Index (SSCI) y Arts & Humanities Citation Index (A&HCI). Abarca más de 12.000 títulos de revistas, 148.000 actas de congresos y 60.000 libros. Su contenido se clasifica en 5 categorías generales, 153 áreas de investigación, que a su vez se descomponen en 254 categorías temáticas.

Otro de los productos que ofrece WoS es el *Journal Citation Reports*<sup>12</sup> (JCR). Es un portal de revistas indexadas en la WoS que determina la importancia relativa de las revistas científicas dentro de una categoría y muestra su factor de impacto, entre otros indicadores. Scimago Journal & Country Rank<sup>13</sup> (SJR) es el otro portal que evalúa revistas y países mediante su propio indicador de impacto (SJR), basado en la información contenida en la base de datos Scopus. Las revistas se agrupan por área temática, categoría temática o país.

## **4.2. Metodología**

La propuesta metodológica presentada en esta tesis se fundamenta en la combinación de distintas técnicas para el previo procesamiento de la información, protocolos de búsqueda e indicadores bibliométricos usando distintos softwares de acceso abierto.

### **4.2.1. Procesamiento de la información**

Con la finalidad de realizar las primeras pruebas para la delimitación de NST, en 2012, se obtuvo un primer conjunto de datos sobre producción científica

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<sup>11</sup> <https://www.webofscience.com/wos>

<sup>12</sup> <https://jcr.clarivate.com/jcr>

<sup>13</sup> <https://www.scimagojr.com>

de NST en la base de datos Scopus, aplicando la estrategia de búsqueda desarrollada en Muñoz-Écija et al. (2013). Para el año 2010, se recuperaron un total de 125.478 documentos. La implementación de estos resultados junto al análisis de citación dio lugar a la primera versión de la categoría temática *Nanoscience and Nanotechnology* en el SJR. Posteriormente, esta metodología se adaptó a otras categorías temáticas que han sido establecidas en este índice de revistas: Social Work<sup>14</sup>, Sports Science<sup>15</sup> y E-learning<sup>16</sup>; categorías temáticas delimitadas en SJR que no contempla la base de datos Scopus.

Para determinar la estructura intelectual y cognitiva (Capítulo 9, primer artículo: *Identification and visualization of the intellectual structure and main research lines in Nanoscience and Nanotechnology at the worldwide level*), se realizó un estudio bibliométrico basado en el análisis de citas y el análisis de copalabras extraídas de la producción científica de NST —198.275 documentos— indexada en la categoría de WoS *Nanoscience & Nanotechnology* (SCI Expanded, en su edición de 2014), para el período temporal 2000-2013. El análisis de citas, para detectar los trabajos elementales de la NST, se llevó a cabo con el uso del programa CitNetExplorer (van Eck & Waltman, 2014). Este programa permite visualizar y analizar redes de citas de publicaciones científicas, identificando grupos de publicaciones estrechamente relacionados. De este modo, se pudo crear y visualizar la red intelectual del dominio científico y las diferentes relaciones entre los distintos grupos identificados.

El análisis de copalabras, extraídas de los títulos y los resúmenes de las publicaciones, se ejecutó con el programa VOSviewer (van Eck & Waltman, 2010). Este software permite generar y visualizar redes bibliométricas sobre la base de citas, emparejamiento bibliográfico, cocitación, relaciones de

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<sup>14</sup> <https://www.scimagojr.com/journalrank.php?category=3323&type=j>

<sup>15</sup> <https://www.scimagojr.com/journalrank.php?category=3699&type=j>

<sup>16</sup> <https://www.scimagojr.com/journalrank.php?category=3399&type=j>

coautoría o coocurrencia de términos. Antes de generar los mapas, se elaboró un tesoro con el fin de estandarizar acrónimos, plurales y singulares, además de eliminar palabras vacías o términos con escaso significado.

Para evitar un ruido excesivo y mostrar solo los términos más significativos, los mapas de copalabras fueron generados con un umbral de ocurrencia igual o mayor a 5 ( $\geq 5$ ). Igualmente, para evitar que se pierda información sobre los frentes de investigación y su evolución, el período temporal se desglosó en 4 intervalos: los dos primeros de cuatro años (2000-2003 y 2004-2007) y los dos últimos de tres años (2008-2010 y 2011-2013) (Vargas-Quesada et al., 2010; Moya-Anegón et al., 2006). En consecuencia, se construyeron cuatro mapas de copalabras acordes a los períodos temporales establecidos.

El conjunto de datos para comparar las diferentes aproximaciones de la delimitación de campos de conocimiento (Capítulo 10, segundo artículo: *Coping with methods for delineating emerging fields: Nanoscience and nanotechnology as a case study*) se recuperó mediante el uso de una estrategia de búsqueda (Capítulo 4, Apartado 4.2.2). En 2017 se lanzó la búsqueda sin aplicar ningún tipo de filtro por tipología documental. Pero debido al gran volumen de documentos recuperados (1.626.360 en Scopus y 1.253.453 en WoS), se aplicó el intervalo temporal 2008-2015. Por tanto, el total de documentos recuperados fue 902.082 en Scopus y 711.464 en WoS.

Al mismo tiempo, para las categorías *Nanoscience and Nanotechnology*, en sus ediciones 2015 y 2016, y *Multidisciplinary*, en todas sus ediciones, se utilizaron los índices de revistas JCR de WoS y SJR para Scopus.

Por otra parte, se amplió el estudio longitudinal de la estructura cognitiva de la NST (Capítulo 11, tercer artículo: *Unveiling cognitive structure and comparative advantages of countries in knowledge domains*). El conjunto de publicaciones utilizadas se recuperó de Scopus, aplicando la estrategia de

búsqueda presentada en Muñoz-Écija et al. (2019). Se tuvieron en cuenta todas las tipologías documentales recuperadas.

Con el fin de poder percibir los cambios producidos en la investigación en NST en la segunda década del siglo XXI, se eligieron tres períodos: 2010, 2014 y 2018. Por último, para poder comparar a España con otros países de la Unión Europea, se filtraron los datos a nivel geográfico y se acotaron a los dos países más productores en NST de la UE: Alemania y Francia. La Tabla 1 muestra el número de total documentos recuperados a nivel global y por países.

**Tabla 1.** Número de publicaciones de Nanociencia y Nanotecnología en Scopus (2010-2014-2018)

	<b>2010</b>	<b>2014</b>	<b>2018</b>
<b>Alemania</b>	7.322	8.584	8.558
<b>Francia</b>	4.818	5.631	5.517
<b>España</b>	2.780	3.808	4.124
<b>Mundo</b>	96.605	136.731	162.914

Para poder comparar estructuras estables, se elaboraron mapas solapados de copalabras con la producción científica de Scopus, para los años 2010, 2014 y 2018.

Las unidades de análisis utilizadas para elaborar los mapas solapados fueron las palabras clave de los documentos, en este caso, *author keywords* e *indexed keywords*. La base de datos Scopus define *author keywords* como “palabras clave elegidas por el autor o autores que, en su opinión, reflejan mejor el contenido de su documento”; y las *indexed keywords* como “palabras clave elegidas por los proveedores de contenido y estandarizadas en base a vocabularios disponibles públicamente. A diferencia de las *author keywords*, las palabras clave indexadas tienen en cuenta sinónimos, diversas grafías y plurales” (Elsevier B.V., 2021). Dicho de otro modo, las *author keywords* son palabras no estandarizadas, procedentes del lenguaje natural, asignadas por los autores para definir el contenido de sus publicaciones. Por el contrario, las

*indexed keyword* son palabras estandarizadas en vocabularios controlados que asignan los proveedores de contenido para definir el contenido de las publicaciones.

Por consiguiente, se generaron mapas base a nivel global para cada uno de los años (2010, 2014 y 2018) con un umbral de coocurrencia mayor o igual a 10 ( $\geq 10$ ). Sobre estos mapas se solaparon los mapas generados para cada uno de los países estudiados (Alemania, Francia y España), mapas con un umbral de coocurrencia mayor o igual a 4 ( $\geq 4$ ).

#### **4.2.2. Protocolos de búsqueda**

La comparativa de diferentes aproximaciones para la delimitación de dominios científicos se realizó a tres niveles de agregación: categorías, revistas y publicaciones (Capítulo 10, segundo artículo: *Identification and visualization of the intellectual structure and main research lines in Nanoscience and Nanotechnology at the worldwide level*).

##### **Aproximación a nivel de categorías**

Este método, que asigna revistas a una categoría basándose en los datos de citación (Pudovkin & Garfield, 2002), se aplica en la base de datos de WoS para delimitar las categorías científicas. Se seleccionaron 88 revistas atendiendo a las revistas incluidas en las versiones JCR de 2015 y 2016 para *Nanoscience & Nanotechnology*.

##### **Aproximación a nivel de revistas**

En esta aproximación se implementó un procedimiento compuesto de 7 pasos, que utiliza el análisis estadístico para estimar algunos de los parámetros.



### Paso 1. Estrategia de búsqueda

Se diseñó una estrategia de búsqueda basada en la combinación del prefijo “nano” y una lista de palabras clave relacionadas con la NST mediante operadores booleanos. Para elaborarla, se compilaron diferentes estrategias de búsqueda de NST previamente publicadas en literatura (Arora et al., 2013; Grieneisen & Zhang, 2011; Kostoff, Koytcheff et al., 2006; Maghrebi et al., 2011).

Para poder trabajar en paralelo con los datos indexados en Scopus y Wos, en 2017, se lanzaron las búsquedas en ambas bases de datos, sin utilizar ningún tipo de filtro por tipología documental.

### Paso 2. Análisis de citas

Se identificaron las revistas citadas en las publicaciones NST recuperadas en cada base de datos. Previamente, el análisis de citas reveló revistas de carácter multidisciplinar incluidas en la categoría *Multidisciplinary* de JCR y SJR. Estas revistas fueron eliminadas ya que no pueden considerarse que pertenezcan a ningún dominio científico específico (Narin, 1976). Asimismo, lo multidisciplinar puede considerarse como un indicador de la dimensión que cita más que de la dimensión citante (Leydesdorff, 2007).

### Paso 3. Criterio del codo (*Elbow criterion*) con umbral de curvatura

Después de haber obtenido el porcentaje de citación de las revistas citadas, se utilizó el *Elbow criterion* (método del codo) para seleccionar las revistas más representativas. La visualización de este método se llevó a cabo empleando un procedimiento estadístico. En concreto, se estimó un modelo con un umbral desconocido de curvatura (Hansen, 2017; Andrews, 1993) y dos líneas rectas conectadas en el punto donde la pendiente de la curva disminuye, basado en el método de Mínimos Cuadrados Ordinarios. Este modelo permitió la mejora del método anteriormente aplicado para determinar

el punto de corte (*cut-off*) (Muñoz-Écija et al., 2013), que era bastante aleatorio.

#### Paso 4. Revistas con prefijo nano

Se ejecutó una búsqueda con el prefijo nano\* en el campo *Source* tanto en Scopus como en WoS. Ambas búsquedas permitieron localizar todas las revistas que contenían el prefijo “nano” en sus títulos. Los títulos recuperados se revisaron para elegir solo las revistas vigentes y descartar las revistas cesadas. Para evitar duplicados, se excluyeron de estas revistas con prefijo “nano” las que habían sido anteriormente identificadas en el paso 3.

#### Paso 5. Compilación de revistas de JCR, SJR y de revistas con prefijo nano

Se seleccionaron todas las revistas incluidas en la categoría *Nanoscience and Nanotechnology* de JCR y SJR, en sus versiones 2015 y 2016. Posteriormente, se agregaron las revistas con prefijo “nano” del paso 4 con el fin de detectar revistas no identificadas en los pasos anteriormente descritos. Para evitar duplicados, se descartaron de esta compilación las revistas que habían sido identificadas en el paso 3. En consecuencia, obtuvimos un grupo de revistas diferentes para los datos de Scopus del que obtuvimos para los datos de WoS.

#### Paso 6. Análisis de citas de las revistas compiladas en el paso 5

En este paso, la finalidad era localizar revistas esenciales que no hubiesen sido reveladas en los pasos previos. En otras palabras, se pretendía conocer a qué revistas citaban las publicaciones de las revistas centrales de NST. Por tanto, se recuperaron las publicaciones de las revistas recopiladas en el paso 5 para ambos conjuntos de datos (Scopus y WoS). A continuación, se realizó un análisis de citas, de igual manera que se realizó en el paso 2.

## Paso 7. Criterio del codo (*Elbow criterion*) con umbral de curvatura

Con el fin de poder seleccionar las revistas más importantes entre las 100 revistas que recibieron más citas en el paso 6, se aplicó de nuevo el *Elbow criterion* con umbral de curvatura. De esta manera, se volvieron a identificar revistas no detectadas en los pasos anteriores.

Por último, aunamos todas las revistas identificadas en los pasos 3, 4 y 7 para cada grupo de datos (Scopus y WoS), dando lugar a dos listas de revistas. Estas listas no mostraron diferencias significativas. Por consiguiente, agregamos las dos listas, obteniendo así el listado final de revistas centrales de NST.

### **Aproximación a nivel de publicaciones**

A partir de una estancia de investigación<sup>17</sup> realizada en el *Centre for Science and Technology Studies* (CWTS) en la Universidad de Leiden, se implementó la aproximación a nivel de publicaciones. En esta aproximación se trabajó con los desarrolladores del Sistema de Clasificación a Nivel de Publicaciones del CWTS, cuya metodología se describe en Waltman y van Eck (2012). Este sistema de clasificación comprende más de 4.100 categorías, también conocidas como campos a nivel micro o microcampos.

Se aplicó la estrategia de búsqueda a la tipología documental usada en este sistema de clasificación: publicaciones y revisiones, y se recuperaron 1.005.801 documentos para los años 2000-2016. Estos documentos se superpusieron en el sistema de microcampos, localizándose en un total de 3.433 microcampos entre 2008-2015. El porcentaje de publicaciones superpuestas se calculó dividiendo el número de publicaciones coincidentes por microcampo por el número total de publicaciones en cada microcampo. Solo se seleccionaron los microcampos con un umbral igual o superior a 0,6

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<sup>17</sup> Movilidad Internacional de Jóvenes Investigadores de Programas de Doctorado de la Universidad de Granada y CEI Bio-Tic para el curso académico 2016-2017.

de publicación superpuesta. Posteriormente, se calculó el número de publicaciones por revista que cubrían los 35 microgrupos seleccionados, así como el número total de publicaciones por revista en la colección de WoS para el mismo período de tiempo. Por tanto, el porcentaje de publicaciones por revista se obtuvo dividiendo estos dos valores. Se extrajeron las revistas con un umbral superior a 0,2 de publicación por revista y más de 50 publicaciones.

### **Consulta a expertos**

La consulta a expertos se realizó a través del envío de una encuesta (Capítulo 10, Appendix A), que resultó fundamental para la interpretación de los mapas y la validación de revistas y artículos en NST. Por un lado, se consultó de manera directa a expertos en NST para corroborar los temas de investigación detectados. Por otro lado, se realizó un cuestionario, gestionado con el software Qualtrics, donde los expertos respondían sobre la idoneidad de una muestra aleatoria de publicaciones para ser consideradas publicaciones de Nanociencia y Nanotecnología.

#### **4.2.3. Indicadores bibliométricos**

Entre los indicadores bibliométricos para el análisis y la caracterización de la NST se utilizaron los detallados a continuación.

#### **Indicadores cuantitativos de la producción científica**

A modo de resumen, los indicadores cuantitativos empleados permitieron:

- medir la cantidad de conocimiento producido a través de las publicaciones y su evolución a lo largo del tiempo;
- determinar los períodos y documentos claves en el desarrollo del dominio científico, su estructura cognitiva e intelectual;

- analizar la especialización temática a nivel de país.

Seguidamente, se describe el significado de cada indicador y el procedimiento de obtención.

**Número de Publicaciones** ( $N_{pub}$ ) (Capítulos 9, 10 y 11): es el valor absoluto del número de documentos de cualquier tipología documental publicados por un dominio científico, en este caso en NST, durante los períodos de tiempo estudiados. Es una medida de magnitud de la producción científica total.

$$N_{pub} = pub_1 + pub_2 \dots pub_n$$

**Porcentaje de Publicaciones** ( $\%N_{pub}$ ) (Capítulos 9, 10 y 11): porcentaje de publicaciones respecto al total de publicaciones de referencia. Esta medida estima el grado de participación de los países o cualquier otro nivel de agregación, en el conjunto total de la producción de publicaciones.

$$\%N_{pub(i)} = \frac{N_{pub_i}}{N_{pub}} * 100$$

**Tasa de Crecimiento** (GR) (Capítulos 9 y 11): presenta la variación en el volumen de producción científica del dominio científico respecto al año previo. La medida es la diferencia porcentual del número de publicaciones con respecto al año anterior. Este indicador se calcula para precisar la evolución de la producción científica del dominio científico a nivel global y nacional.

$$GR_t = \left( \frac{N_{pub_t}}{N_{pub_{t-1}}} - 1 \right) * 100$$

**Tasa Promedio de Crecimiento** (MAGR) (Capítulos 9 y 11): expresa los crecimientos promedio de la producción científica durante varios períodos de tiempo, mostrando los cambios en la actividad de producción científica. Esta medida es la media aritmética de una serie de tasas de crecimiento.

$$MAGR = \frac{GR_1 + GR_2 + \dots + GR_n}{N}$$

**Índice de Actividad (AI)** (Capítulo 11): conocido también como Índice de Especialización (Frame & Carpenter, 1979), denota el esfuerzo de investigación relativo que un país dedica a un dominio científico determinado. Este indicador permite cuantificar en qué medida un país contribuye a la producción científica de un determinado dominio científico a nivel mundial. En esta investigación, la siguiente fórmula se utilizó para determinar la especialización de los países en la producción científica de NST.

$$AI = \frac{\%NPub_{NST} (country)}{\%NPub_{NST} (world)}$$

Cuando el AI es mayor que 1 ( $AI > 1$ ) significa que la producción científica del país en Nanociencia y Nanotecnología es más alta que el promedio mundial. Por el contrario, si los valores de este indicador son menores o iguales que 1 ( $AI \leq 1$ ) implica una menor producción científica en NST que el promedio mundial.

**Índice de Especialización Relativa (RSI)** (Capítulo 11): convierte los valores del Índice de Actividad en una escala entre -1 y +1 (Glänzel, 2000). De este modo, posibilita comparar a los países con el fin de evaluar las fortalezas relativas de cada país en un dominio científico dado. En este caso, el dominio científico NST.

$$RSI = \frac{AI - 1}{AI + 1}$$

Por tanto, cuando  $RSI > 0$  indica especialización científica de un país en NST sobre la base del mundo, representada por el valor 0. Si  $RSI < 0$  expresa la no especialización de un país en este dominio científico.

**Índice de Actividad de Palabras Clave (KAI)** (Capítulo 11): expresa la ventaja comparativa que tiene un país en un determinado tema de investigación. Este indicador es una variante del AI, pero tomando como unidad de análisis palabras clave (Chen et al., 2015). El KAI ha sido calculado teniendo en cuenta dos parámetros: el número total de palabras claves y el número total de ocurrencias (número total de publicaciones en las que aparecen las palabras clave).

KAI

$$= \frac{\text{porcentaje de un tema de investigación específico en las palabras clave del país}}{\text{porcentaje de un tema de investigación específico en el total de palabras clave a nivel mundial}}$$

Esta fórmula puede expresarse también de la forma:

$$KAI = \frac{\left( \frac{n(k, d, c)}{n(d, c, all)} \right) * 100}{\left( \frac{n(k, d)}{n(d, all)} \right) * 100}$$

donde  $n(k, d, c)$  denota el número de publicaciones donde aparece una palabra clave o sintagma nominal ( $k$ ) en un dominio científico específico ( $d$ ) para un país concreto ( $c$ );  $n(d, c, all)$  denota el número total de palabras clave en un dominio científico específico ( $d$ ) para un país concreto ( $c$ );  $n(k, d)$  denota el número de publicaciones donde aparece una palabra clave o sintagma nominal ( $k$ ) en un dominio científico específico ( $d$ ) a nivel mundial;  $n(d, all)$  denota el número total de palabras clave a nivel mundial en un dominio científico específico.

De igual manera, la fórmula también se utilizó teniendo en cuenta el número total de ocurrencias de las palabras clave. En otras palabras, el divisor es el número total de publicaciones que contienen palabras clave. Por tanto, se calculó el KAI atendiendo al número total de ocurrencias de NST.

**Índice de Especialización Relativa de Palabras Clave (RSIk)** (Capítulo 11): al igual que el Índice de Especialización Relativa, permite transformar los valores del KAI en valores entre -1 y +1. Esta transformación posibilita la comparativa entre los diferentes países y temas de investigación del dominio científico. Los valores superiores a 0 indican una ventaja competitiva con respecto al mundo. Por el contrario, los valores inferiores a 0 no evidencian ventaja competitiva.

El número total de términos permite identificar aquellas temáticas que presentan una mayor especialización con respecto al mundo y refleja el énfasis que la comunidad científica pone en ellos. Al discriminar la frecuencia como denominador, podemos detectar la especialización de términos que, a pesar de tener valores bajos de frecuencia, muestran una ventaja competitiva. Estos términos pueden expresar nuevos conceptos que emergen de un campo temático o temas de innovación. Por tanto, este indicador facilita conocer mejor una temática, la especialización a nivel mundial y cómo evolucionan a lo largo de los años. Por el otro, al analizar el RSIk en función del número total de frecuencias de los términos puede denotar palabras que son muy populares dentro del dominio científico, pero excluir otras que pueden ser buenas representantes de la especialización.

**Número de Citas Recibidas** (Capítulos 9 y 10): indica el valor absoluto del número de citas que una revista ha recibido por un grupo de publicaciones, en este caso, la producción científica de NST. Asimismo, las publicaciones citantes de la producción científica analizada determinan las revistas más citadas en NST, desvelando sus patrones de citación.

$$N_{citations_j} = citation_1 + citation_2 \dots citation_n$$

**Citation-Assisted Background (CAB)** (Capítulo 9): este indicador permite identificar los documentos clave de un dominio científico a través de análisis de citas (Kostoff & Shlesinger, 2005). Parte de la idea de que los documentos



determinantes en un dominio científico tienden a recibir muchas citas por parte de comunidad científica en activo, otorgando un cierto valor cualitativo a la hora de evaluar las publicaciones (Cole, 1989; MacRoberts & MacRoberts, 1989; Garfield, 1979). En otras palabras, este indicador considera que existe una relación intelectual entre las publicaciones citadas y las citantes, señalando la influencia que ejercen en la comunidad científica.

Este análisis cuenta el número de citas que ha recibido una publicación en un determinado intervalo temporal. Los factores a tener en cuenta para la aplicación de este indicador son: la clara definición del dominio científico; los documentos que lo componen; la identificación de las referencias citadas con más frecuencia; y la integración y análisis de esas referencias o trabajos más citados dentro de una narración cronológica con la finalidad de explicar los antecedentes del campo de conocimiento.

En esta investigación solo se tuvieron en cuenta las citas recibidas por las revistas de la categoría *Nanoscience & Nanotechnology* de JCR edición 2014.

**Porcentaje de Citas por Revista** (Capítulo 10): determina el porcentaje de citas que ha recibido una revista con respecto al total de la citación de las publicaciones de referencia. El indicador es el cociente del número de citas que ha recibido una revista entre el número total de citas recibidas.

$$\%Ncitations_{(j)} = \frac{Ncitations_j}{\sum Ncitations} * 100$$

**Coocurrencia de palabras** (Co-words) (Capítulo 9 y 11): hace referencia a la frecuencia de aparición de dos términos de un corpus temático a una cierta distancia. La proximidad entre los términos se traduce en una estrecha relación entre los mismos (Callon et al., 1991). Además, la coocurrencia asume la interdependencia de los dos términos.

**Precisión y Exhaustividad** (Capítulo 10): estos parámetros han sido tradicionalmente utilizados para medir la efectividad de los sistemas para recuperar información y establecer comparaciones entre ellos (Chowdhury, 2010) .

La precisión hace referencia a la proporción de documentos recuperados que son relevantes. La exhaustividad es la proporción de material relevante recuperado en un sistema de información, por ejemplo, una base de datos. Los valores de estos parámetros son expresados en valores relativos, representando el valor 1 el valor máximo de precisión y exhaustividad (Salton & McGill, 1983).

En esta investigación, estos parámetros han sido alterados para poder aplicarlos. Por un lado, la precisión máxima viene determinada por la definición de nanotecnología de la *National Nanotechnology Initiative* (NNI) de los Estados Unidos. De este modo, se determinó la precisión a dos niveles: revistas y publicaciones. En el caso de las revistas, la precisión se estimó considerando cómo se ajustaban las descripciones de las revistas en sus secciones *Objetivo y Alcance* y *Descripción general* a la definición de nanotecnología de la NNI. Se confeccionó una escala entre 0 y 1 atendiendo a los siguientes valores:

- 1 = Revistas que cubren solo temas de NST
- 0.5 = Revistas que cubren temas de NST junto a otros temas
- 0 = Revistas que no cubren temas de NST

A continuación, se calculó el promedio de los valores de precisión para cada una de las aproximaciones.

$$Precision (\bar{x}) = \frac{\sum_{i=1}^n x_i}{n}$$

La precisión para las publicaciones se calculó analizando las respuestas de los cuestionarios enviados a expertos en NST. Se atribuyó el valor 1 a las publicaciones que los expertos definieron como relevantes y 0 a las que no fueron definidas como relevantes.

Por otra parte, la exhaustividad se calculó también para las revistas y para las publicaciones. En el caso de las revistas, se determinó al total de revistas identificadas en las tres aproximaciones como la exhaustividad máxima. Con las publicaciones, la exhaustividad se calculó asumiendo que todas las publicaciones de la muestra representaban la exhaustividad máxima y estimamos como publicaciones relevantes todas aquellas que hubiesen sido validadas por los expertos con una precisión igual o superior a 0.5.

**Fleiss's kappa** (Capítulo 10): es una medida estadística que evalúa el nivel de concordancia entre evaluadores al clasificar elementos (Fleiss, 1971). Este valor relativo oscila entre -1 y +1, donde 0 representa la concordancia esperada y 1 representa la concordancia perfecta entre expertos. Se utilizaron las pautas de Landis y Koch (1977) para interpretar los valores de este indicador.

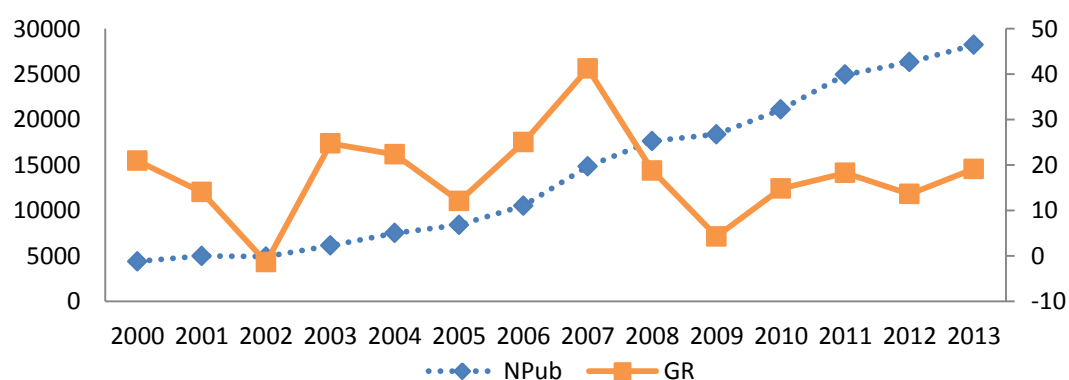
## Capítulo 5. Resultados y discusión

En este capítulo se presenta un compendio general de los resultados más relevantes de cada una de las publicaciones.

### 5.1. Estructura intelectual y cognitiva de Nanociencia y Nanotecnología a nivel mundial

*¿Cuál es la estructura intelectual de la NST? ¿Cuál es la estructura cognitiva? ¿Cuál ha sido su evolución temática? (Capítulo 9)*

La Figura 2 muestra la evolución del número de documentos indexados en la categoría *Nanoscience & Nanotechnology* de la WoS entre 2000 y 2013 (198.275 publicaciones). La producción científica tiende a crecer a lo largo de los años de estudio con distintos ritmos. Se puede observar que el mayor crecimiento se produjo entre los años 2004 y 2007 (102,17%), justo después del Nobel sobre grafeno. En 2009, se apreció un descenso relativo (4,26%), volviendo a mostrar valores más estables a partir de 2010 y 2013 (14,79%, 18,27%, 13,61% y 19,14%).



**Figura 2.** Evolución de la producción científica en la categoría Nanociencia y Nanotecnología en WoS.

Leyenda: La línea de color azul indica el número de publicaciones recuperadas la categoría NST de WoS. La línea naranja indica la tasa de crecimiento anual de las publicaciones.

El análisis de citas de las publicaciones influyentes (*seminal papers*) facilitó generar una representación gráfica de la base de conocimiento de NST, compuesta por 80 nodos (Figura 2, Capítulo 9). Estos nodos fueron citados al menos 600 veces por la producción científica NST (2000-2013).

La representación gráfica de la red de publicaciones más influyentes se dividió en 7 grupos diferentes (Figuras 3-6, Capítulo 9). La Tabla 2 muestra los 7 clústeres en los que se concentra la estructura intelectual de NST y el número de nodos que conforma cada uno de ellos. Destacaron los clústeres relacionados con el desarrollo de los *Materiales de carbono (Carbon nanomaterials)* y la *Nanoquímica y Nanomedicina (Nanotechnology and Nanomedicine)*. En estos mismos clústeres se encontraban el mayor número de publicaciones esenciales en el desarrollo de las NST, como es el caso de los artículos relacionados con la invención de los nanotubos de carbono y el grafeno.

Por otro lado, el análisis de copalabras identificó hasta 7 frentes de investigación en distintos períodos temporales: 2000-2003, 2004-2007, 2008-2010 y 2011-2013 (Tabla 2). La exploración de los diferentes mapas de copalabras favoreció la caracterización y comparación de la evolución de los frentes de investigación que componen la estructura cognitiva de la NST a nivel mundial (Capítulo 9, Tablas 1 y 2).

La Figura 3 muestra los mapas de copalabras para cada uno de los períodos. Para el período 2000-2003, el mapa reveló 5 clústeres que corresponden de manera razonable con los frentes de investigación de NST (6.189 términos); entre 2004-2007, el mapa con 14.316 términos mostró 5 frentes de investigación; entre 2008-2010, el mapa con 20.709 términos reveló 6 frentes de investigación; por último, entre 2011-2013, el mapa con 30.137 términos ofreció 5 frentes de investigación.

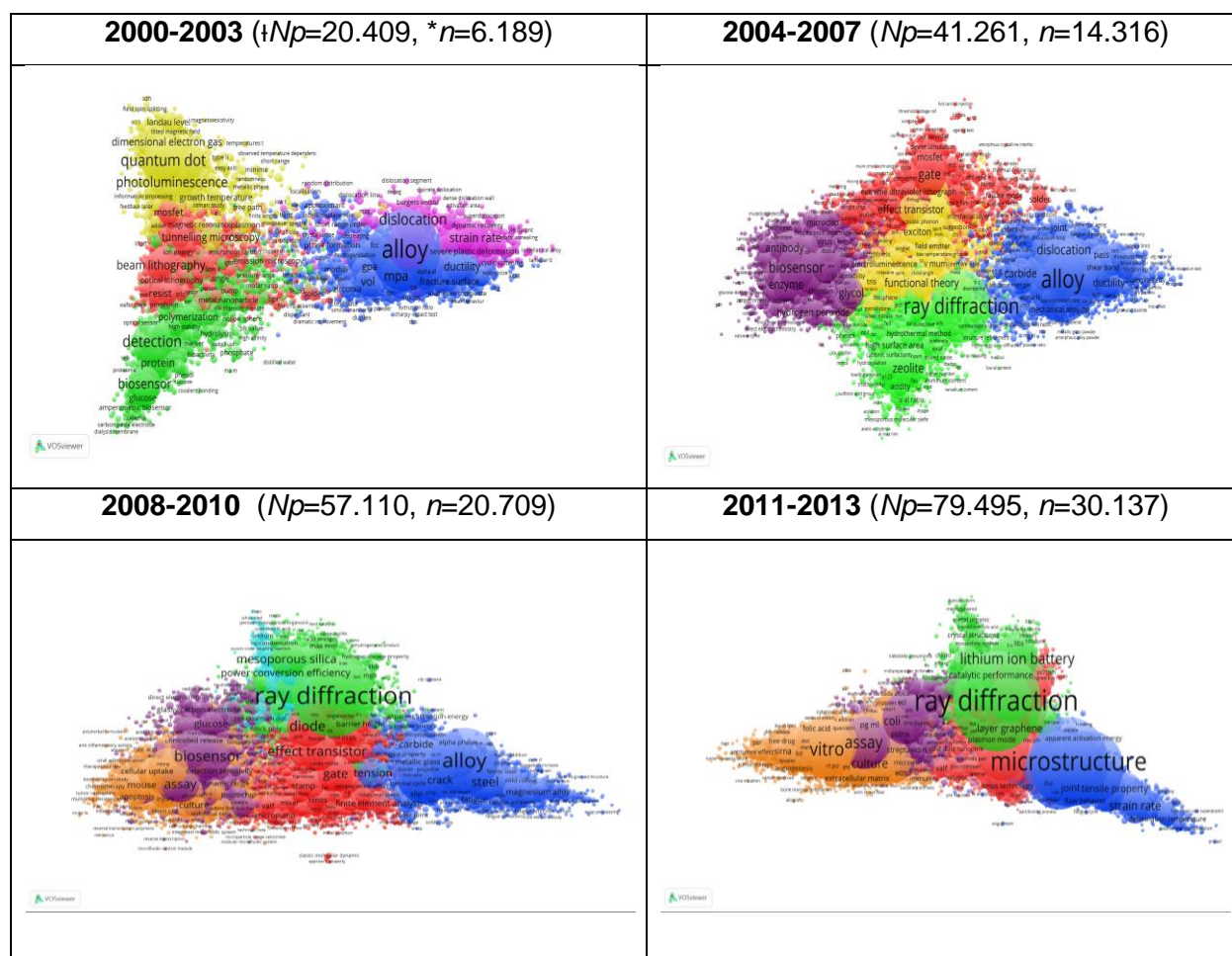
**Tabla 2.** Temáticas que componen la estructura intelectual y cognitiva de NST en WoS

Estructura intelectual		Estructura cognitiva	
Color	Clúster	Color	Clúster
Verde	Carbon nanomaterials (*n=23)	Rojo	Microelectronics Engineering and Top-down Processes
Azul	Nanochemistry and Nanomedicine (n=21)	Verde	Synthesis of Nanomaterials and Bottom-up Processes
Marrón	Physics and Chemistry (n=18)	Amarillo	Optics and Electronics
Naranja	Nanomaterials Characteristics and Manufacturing Techniques (n=13)	Azul	Mechanical Characteristics of Nanomaterials Physical Characteristics of Nanomaterials
Rosa	Nanocatalysis (n=3)	Rosa	
Amarillo	Semiconductor Devices (n=1)	Morado	Biotechnology and Biomedicine: Biosensing
Azul claro	Organic Electronics (n=1)		Naranja
		Azul claro	Organic Electronics

\*n=nodos

A modo general, se apreciaron claras diferencias de configuración de los frentes de investigación. Entre 2000-2003, *Síntesis de Nanomateriales y Procesos Bottom-up e Ingeniería Microelectrónica y Procesos Top-down* mostraron los términos con el mayor promedio de impacto de citas de las publicaciones (Tablas 3-8, Capítulo 9). Además, muchos de los nodos de estos frentes de investigación ocuparon posiciones centrales del mapa, localizándose el resto de clústeres temáticos en posiciones más periféricas

(Óptica y Electrónica, Características Físicas de los Nanomateriales y Características Mecánicas de los Nanomateriales). Estos clústeres reflejaron una indudable definición per se, pues muchos de sus términos tenían frecuencias altas. Sin embargo, se apreció falta de relación entre los clústeres dedicados al estudio de la ciencia básica (izquierda) y la ciencia aplicada (derecha) de la NST.



\* $n$ = Número de nodos

$\dagger N_p$ = Número de publicaciones

**Figura 3.** Mapas de términos de Nanociencia y Nanotecnología (N&N WC 2000-2013)

Nota: Mapas basados en el análisis de copalabras y sus relaciones. La visualización se realizó con el software VOSviewer, aplicando una frecuencia  $\geq 5$  y un algoritmo de clustering con valor 10.

Entre 2004-2007, el frente de investigación *Óptica y Electrónica* evolucionó hasta ocupar la posición central del mapa; los relacionados con las características de los nanomateriales convergieron en un solo clúster; un nuevo frente emergió relacionado con la investigación en *Biotecnología y Biomedicina*; y, por último, se evidenció que los términos que subyacen de publicaciones más citadas provenían de los frentes *Óptica y Electrónica* y *Biotecnología y Biomedicina*.

El tercer período, 2008-2010, destacó por la aparición de un nuevo frente de investigación, la fusión y fragmentación de otros frentes y la consolidación del resto. El clúster *Síntesis de Nanomateriales y Procesos Bottom-up* se fusionó con el clúster *Óptica y Electrónica*, ocupando una posición central del mapa. El clúster *Biotecnología y Biomedicina* se fragmentó en dos: la investigación dedicada a la *Biodetección* y la investigación en *Biomedicina Terapéutica*. También apareció un nuevo frente en la parte superior central del mapa, enfocado en el estudio de la *Electrónica Orgánica* y muy relacionado con *Síntesis de Nanomateriales y Procesos Bottom-up*. La presencia, sin ninguna variante, del resto de clústeres confirma la consolidación de los frentes de investigación *Ingeniería Microelectrónica y Procesos Top-down* y *Características Físicas y Mecánicas de los Nanomateriales*. En este período, destacaron, por su nivel de relevancia, los términos de los frentes *Biotecnología y Biomedicina*, *Síntesis de Nanomateriales y Procesos Bottom-up* junto a *Óptica y Electrónica* y *Electrónica Orgánica*.

En el último período (2011-2013), prevalecieron todos los frentes de investigación presentes en el período previo, a excepción del clúster *Electrónica Orgánica*, que fue absorbido por el frente de investigación *Ingeniería Microelectrónica y Procesos Top-down*. El resto de las temáticas mostraron términos con un destacable peso en la investigación en NST, pero las relaciones fueron disminuyendo, como el caso de *Características Físicas y Mecánicas de los Nanomateriales* y *Biomedicina Terapéutica*. Volvieron a destacar los términos de los frentes de investigación en *Ingeniería*



*Microelectrónica y Procesos Top-down y Biotecnología y Biomedicina* como los términos más relevantes.

En general, la caracterización de los frentes de investigación manifestó una gran actividad y dinamismo de la investigación en *Biotecnología y Biomedicina*. Otros frentes de investigación se fusionaron con frentes más consolidados. Por ejemplo, *Síntesis de los Materiales y Procesos Bottom-up* se fusionó con el clúster *Óptica y Electrónica*. De igual manera, la investigación relacionada con las *Propiedades Físicas y Mecánicas de los Nanomateriales* perdió solidez con respecto al período anterior, dando lugar a un único clúster que se va aislando del resto. Por tanto, estas características determinan la continuidad o no de algunos de sus frentes de investigación y la aparición de los nuevos, así como las palabras/términos con mayor frecuencia para cada uno de los frentes.

Ofrecer una imagen mundial, tanto de la estructura intelectual como de la evolución de la estructura cognitiva NST, evidencia el dinamismo de la disciplina y el desarrollo de tendencias en la investigación (Figura 3). Este hallazgo permite reafirmar que la NST es una disciplina joven con un marcado carácter interdisciplinar, donde convergen conocimientos de muchos campos como la física, la química, la ciencia de los materiales, la biología o la ingeniería (Finardi & Lamberti, 2021). Al mismo tiempo, los análisis de los mapas arrojan información que permite a la comunidad científica conocer las fuentes de conocimiento esencial en el desarrollo de la NST, cómo se han desarrollado los diferentes frentes de investigación que la componen y las dinámicas de su evolución temporal.

## 5.2. Delimitación temática de Nanociencia y Nanotecnología

*¿Cuáles son las cuestiones a tener en cuenta a la hora de la delimitación de dominios científicos emergentes? (Capítulo 10)*

La propuesta metodológica planteada en el Capítulo 10 permite explorar la delimitación temática de la NST, a nivel de publicaciones y de revistas, y su comparación con otras aproximaciones propuestas en la literatura. En concreto, se usan las revistas incluidas en la categoría *Nanoscience & Nanotechnology* del JCR ( $A_1$ ), la propuesta metodológica para la clasificación por revistas ( $A_3$ ) y la clasificación a nivel de publicaciones propuesta por el CWTS ( $A_2$ ). De este modo, se emplean tres niveles de agregación: categoría, revista y publicación.

Los resultados obtenidos en cada una de las aproximaciones empleadas mostraron diferencias tanto en el número de revistas ( $A_1=86$ ,  $A_2=76$ ,  $A_3=113$ ), en el número de documentos identificados por cada una de ellas ( $A_1=291.534$ ,  $A_2=332.784$ ,  $A_3=768.667$ ), así como en los niveles de precisión y exhaustividad (Tabla 3). Los niveles de precisión y exhaustividad en cada una de las aproximaciones alcanzaron su mayor valor, 0,89 y 0,69 respectivamente, en la *aproximación para delimitar a nivel de revistas* ( $A_3$ ). Sin embargo, el valor de precisión para cada una de las aproximaciones en función del conjunto de los documentos identificados indicó el mayor valor en la *aproximación a nivel de publicaciones* ( $A_2=0,62$ ), mientras que la exhaustividad alcanzó el mayor valor (0,56) en la *aproximación a nivel de revistas* ( $A_3$ ). No obstante, ni el número de revistas, ni los valores de precisión y exhaustividad revelaron diferencias de gran consideración.

**Tabla 3.** Número de revistas, de publicaciones, y valores de precisión y exhaustividad para cada aproximación metodológica

	Revistas identificadas	Publicaciones identificadas	Precisión revistas	Exhaustividad revistas	Precisión publicaciones	Exhaustividad publicaciones
A <sub>1</sub>	86	291.534	0,87	0,54	0,47	0,34
A <sub>2</sub>	76	332.784	0,86	0,47	0,62	0,34
A <sub>3</sub>	113	768.667	0,89	0,69	0,56	0,46

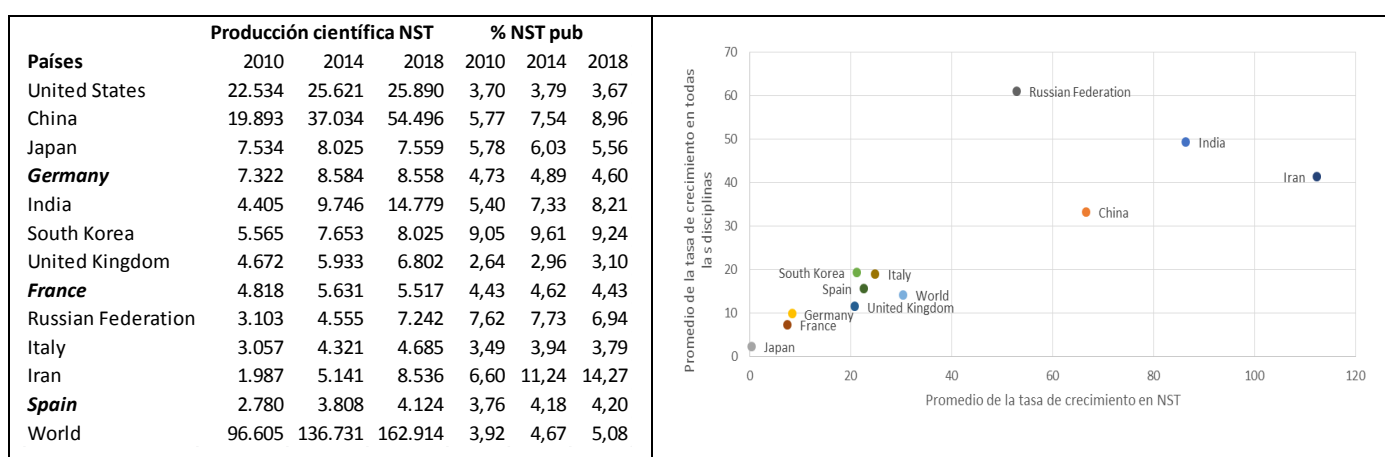
Asimismo, la consulta con los expertos en NST, realizada a través del envío de un cuestionario, plasmó un gran nivel de desacuerdo entre las respuestas a la hora de decidir qué publicaciones deberían de estar contempladas dentro de las publicaciones de NST y las que no. Según el coeficiente kappa de Fleiss, el nivel de acuerdo presentó un valor de 0,27, siendo los expertos en las áreas de NST relativas a física y la química los que mostraron los valores más altos (0,31 y 0,26 respectivamente) (Tabla 3, Capítulo 10).

Por otra parte, los mapas de cocitación de las revistas detectadas en cada una de las aproximaciones empleadas presentaron 4 agrupaciones distintas (Figura 8, Capítulo 10). El clúster rojo, que ocupa la posición central de la red, con revistas especializadas en nanociencia y nanotecnología. A la izquierda, el clúster verde engloba revistas relacionadas con la física. A la derecha, se posicionaron las revistas enfocadas en química. Localizado en la parte inferior de la red, en el clúster amarillo se encontraron las revistas relacionadas con micro y nanoingeniería. La aproximación a nivel de revistas (A<sub>3</sub>) cubrió el mayor número publicaciones en revistas con impacto.

### **5.3. Especialización y ventaja competitiva de Nanociencia y Nanotecnología**

*¿Cómo podemos identificar y rastrear la producción y especialización/competitividad de un dominio científico a nivel mundial y nacional? (Capítulo 11)*

A partir de la estrategia de búsqueda descrita en el Capítulo 10, se descargó la producción mundial de NST con la finalidad de analizar un conjunto de países en Scopus. A nivel mundial, esta producción indicó un crecimiento anual del 30% (2010-2018). Sin embargo, a nivel nacional, el crecimiento de los países no fue homogéneo, ya que algunos países como Irán, India o China aumentaron su producción mucho más que el resto de países estudiados (Figura 4). Estos resultados ponen de manifiesto las diferentes dinámicas y procesos de producción de la NST según el país donde se produce (Chinchilla-Rodríguez et al., 2016).



**Figura 4.** Porcentaje de publicaciones en NST a nivel mundial y nacional en 2010, 2014 y 2018 (izquierda) y promedio de la tasa de crecimiento en NST y en todas las disciplinas (derecha)

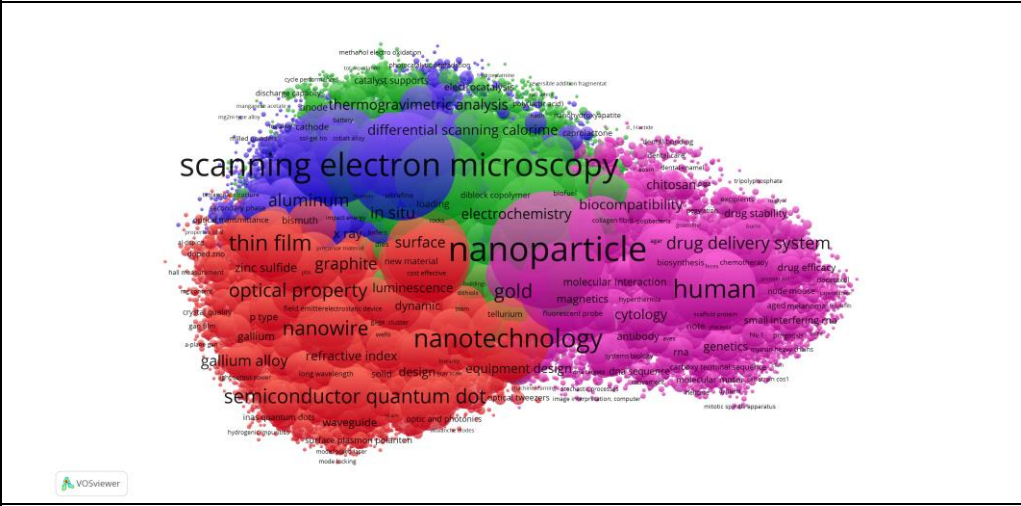
A nivel mundial, el estudio longitudinal de los mapas de copalabras reveló 4 frentes de investigación en el primer período de estudio (2010), llegando a detectarse hasta 6 en el resto de períodos (2014 y 2018). La Tabla 4 muestra los frentes de investigación identificados a través del análisis de clúster. Los frentes de investigación que experimentaron un mayor desarrollo fueron los relacionados con la investigación en nano aplicaciones y dispositivos. Esto sugiere que hay una transferencia del conocimiento básico a la ciencia aplicada con el desarrollo de productos y tecnologías que se ponen a disposición del mercado y de la sociedad. Mientras que el frente de investigación *Características Físicas y Mecánicas de los Nanomateriales* se localiza en la parte central del mapa en los años 2014 y 2018.

**Tabla 4.** Temáticas que componen la estructura cognitiva de NST (Scopus)

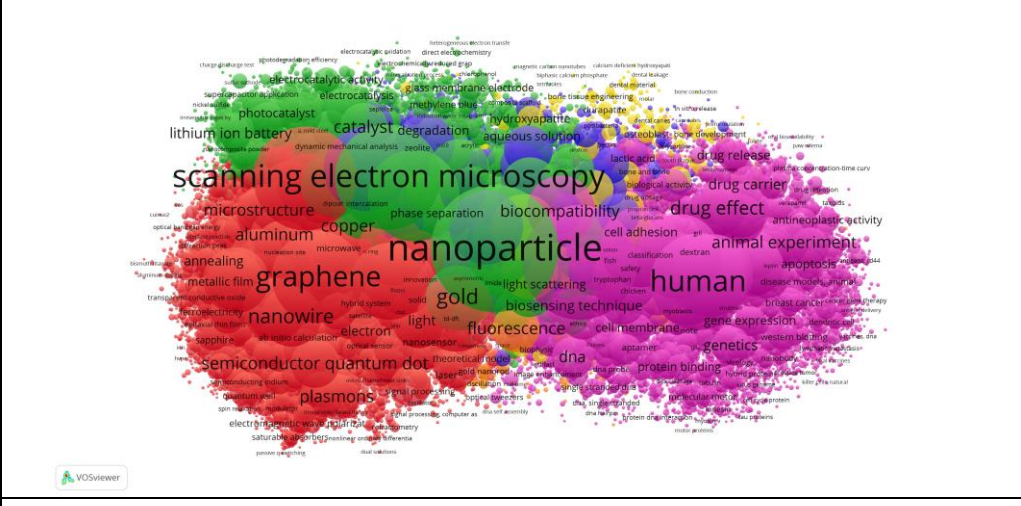
Estructura cognitiva				
Color	Clúster	2010	2014	2018
<b>Rojo</b>	Microelectronics Engineering and Top-down Processes	x	x	x
<b>Verde</b>	Synthesis of Nanomaterials and Bottom-up Processes + Optics and Electronics	x	x	x
<b>Azul</b>	Physical and Mechanical Characteristics of Nanomaterials	x	x	x
<b>Morado</b>	Biotechnology and Biomedicine (BB)	x	BB: Therapeutic Biomedicine	x
			BB: Biosensing	x
			BB: Regenerative Medicine	x

A nivel de país, se aprecian diferencias significativas entre los distintos frentes de investigación a nivel de cohesión (Figura 5). Los tres países analizados, Alemania, Francia y España, mostraron un considerable incremento en la investigación en *Ingeniería Microelectrónica y Procesos Top-down* y, por otra parte, en *Biología y Biomedicina*, especialmente en *Biología Terapéutica*. Pero en España los términos que conforman los mapas muestran una mayor relación entre sí a lo largo del tiempo, lo que sugiere que se investiga con más intensidad.

**2010 (25.407 términos)**



**2014 (22.769 términos)**



**2018 (29.142 términos)**

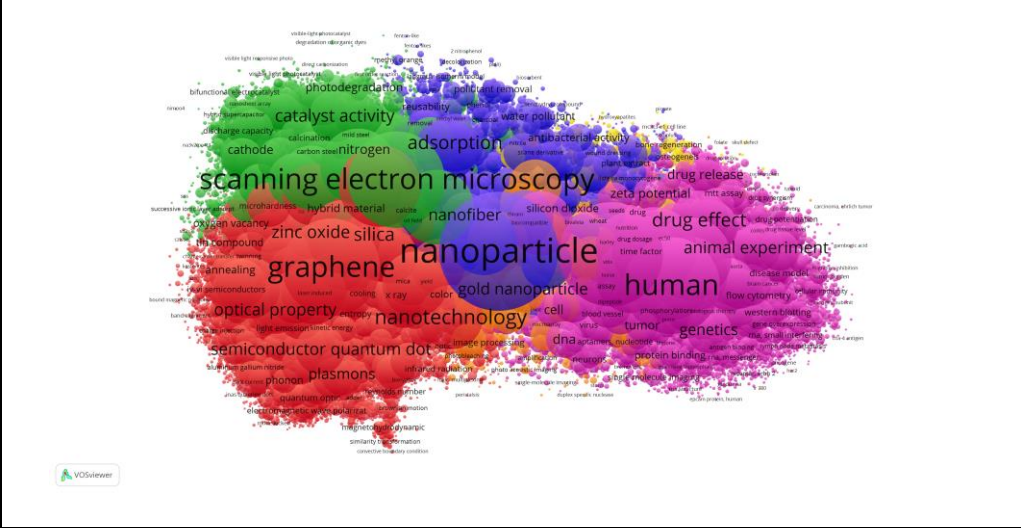
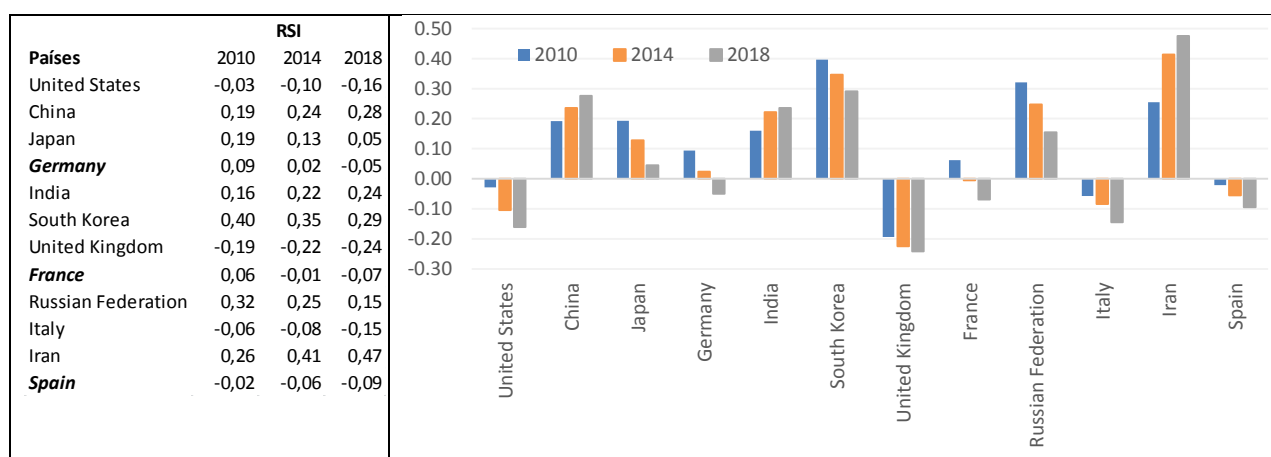


Figura 5. Mapas globales de copalabras de NST (Scopus)

Asimismo, el análisis de los perfiles de especialización desde una doble perspectiva (uso de publicaciones y palabras clave como unidades de análisis) evidenció el esfuerzo relativo que presentan los países en torno a la producción científica de la NST con respecto a la producción mundial. Estados Unidos, Reino Unido y los países más productivos de NST de la UE (Alemania, Francia y España) sufrieron una disminución progresiva en el nivel de especialización, probablemente debida al crecimiento que experimentaron otros como China, India e Irán (Figura 6).



**Figura 6.** Índice de Especialización Relativa de los países más productivos en NST entre 2010 y 2018

De la misma forma, la especialización con base al número de términos y al número de ocurrencias (RSIk) reflejó notables diferencias (Figura 7). La especialización temática en base al número de términos, para Alemania, Francia y España, en todos los frentes de investigación, es menor que la media mundial. Es decir, hay países donde la investigación es mucho más intensa, especialmente en *Síntesis de Nanomateriales y Procesos Bottom-up junto a Óptica y Electrónica y Características Físicas y Mecánicas de los Nanomateriales* (Tabla 1, Capítulo 11). Por el contrario, los mayores esfuerzos se produjeron en la investigación en ingeniería electrónica y biotecnología. Los resultados revelaron la tendencia hacia la exploración de tecnologías y aplicaciones, debido al remarcable potencial que supone para biomedicina. Destacó *Biomedicina Terapéutica* como el frente de

investigación más competitivo en Alemania y España con respecto al mundo, siendo España la más ventajosa. Asimismo, España también destacó en *Medicina Regenerativa*. En cambio, Francia está más especializada en *Ingeniería Microelectrónica y Procesos Top-down*.

Cuando necesitamos conocer cómo las temáticas de un dominio se relacionan entre sí, la combinación de las técnicas de mapeo de la estructuras cognitivas resultan fundamentales (Bu et al., 2020). Los resultados revelaron la tendencia hacia la exploración de nuevas tecnologías y aplicaciones, debido al remarcable potencial que supone para la industria y la sociedad (Cozzens et al., 2013; Roco et al., 2011) y al desarrollo de la ciencia básica del campo de conocimiento (Porter et al., 2019).

Por otro lado, mientras la especialización disminuye en algunos países, como ocurre en Alemania y Francia, aumenta en otros como Irán y China (Figura 4 y 6). En consecuencia, los perfiles de especialización pueden ser altos a pesar de una baja producción a nivel mundial (Figura 6). Así, la dinámica de la producción científica en cada país y las interacciones entre países son factores determinantes para los avances en NST u otros campos de especialización (Chinchilla-Rodríguez et al., 2016).

Comparar la estructura cognitiva de NST a nivel nacional destaca las fortalezas de los países. Este proceso facilita tener información que puede ser usada para orientar la investigación hacia determinados campos de investigación, mantener una posición estable de las temáticas de investigación en las que los países destaquen o crear alianzas o vínculos de colaboración con otros estados y compensar las debilidades detectadas.

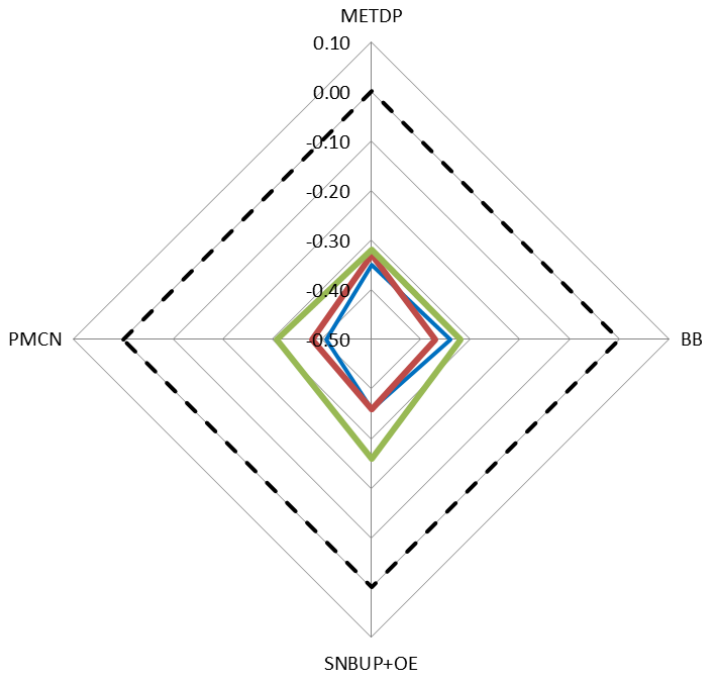
Los entornos institucionales y la gestión de la investigación pueden desempeñar un papel clave en estos resultados. Se necesita un análisis más detallado para explorar esta posibilidad.



**2010**

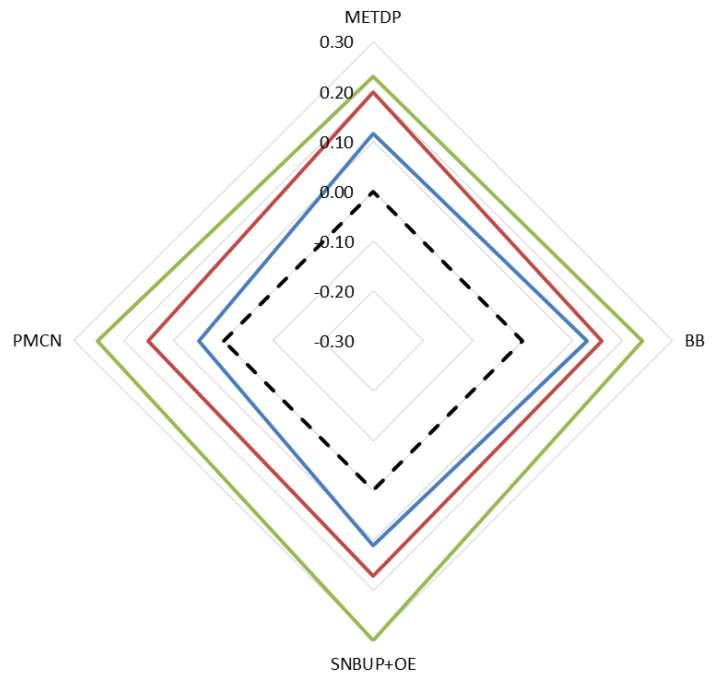
Número de términos

Mundo 247.710; Alemania 37.219; Francia 27.914 ; España 19.391



Número de coocurrencias

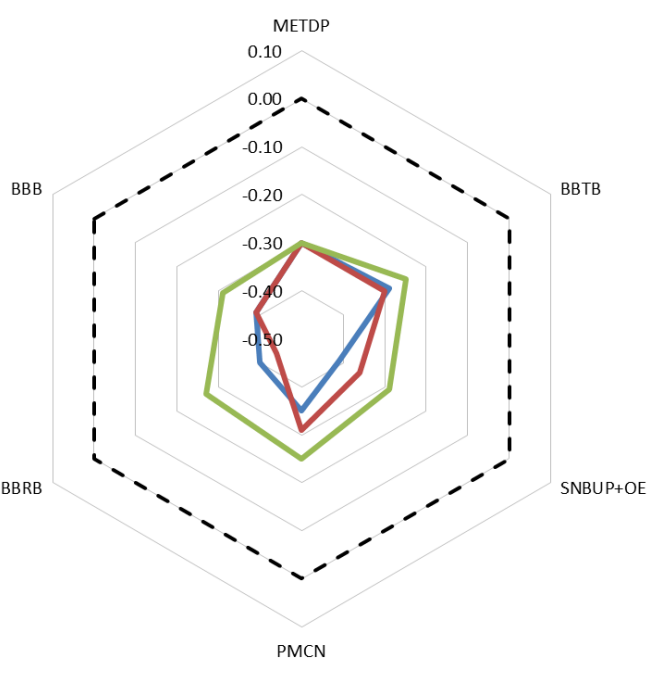
Mundo 2.147.313; Alemania 111.814; Francia 72.407 ; España 46.160



**2014**

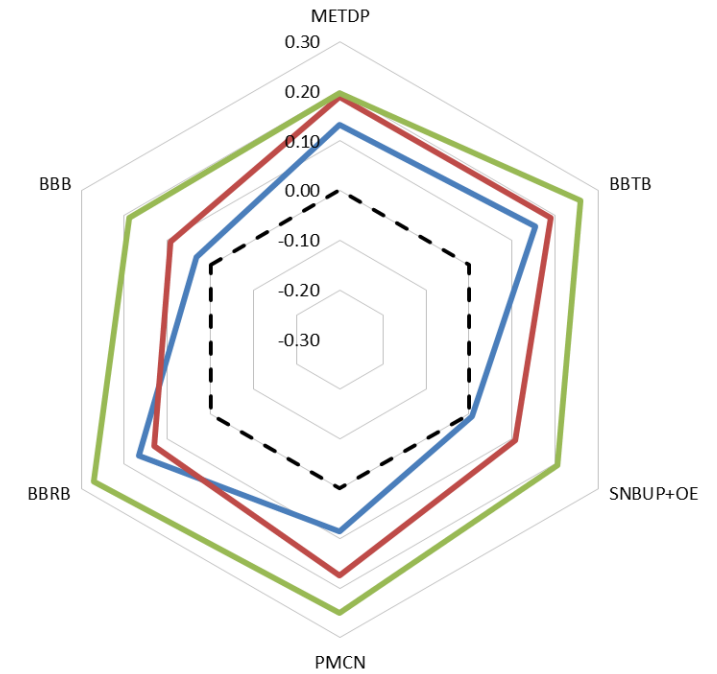
Número de términos

Mundo 273.348; Alemania 35.971; Francia 27.529 ; España 21.271



Número de coocurrencias

Mundo 2.216.954; Alemania 108.832; Francia 74.495 ; España 54.801



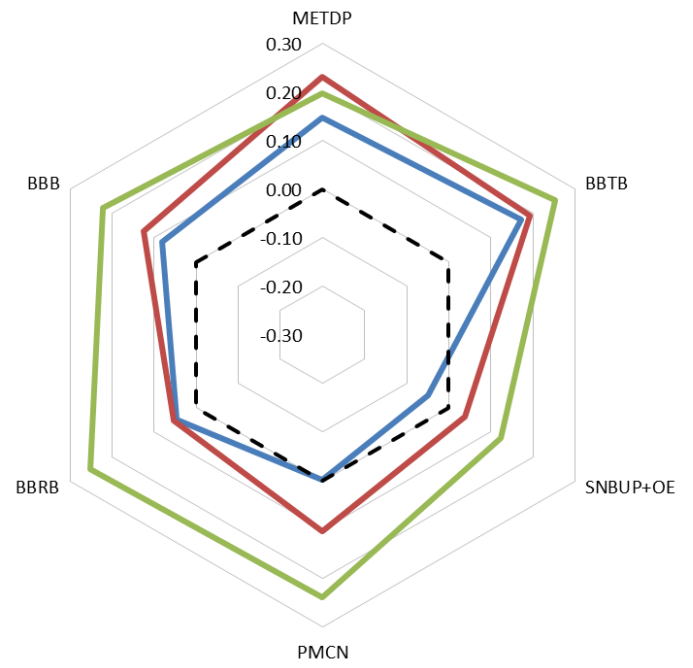
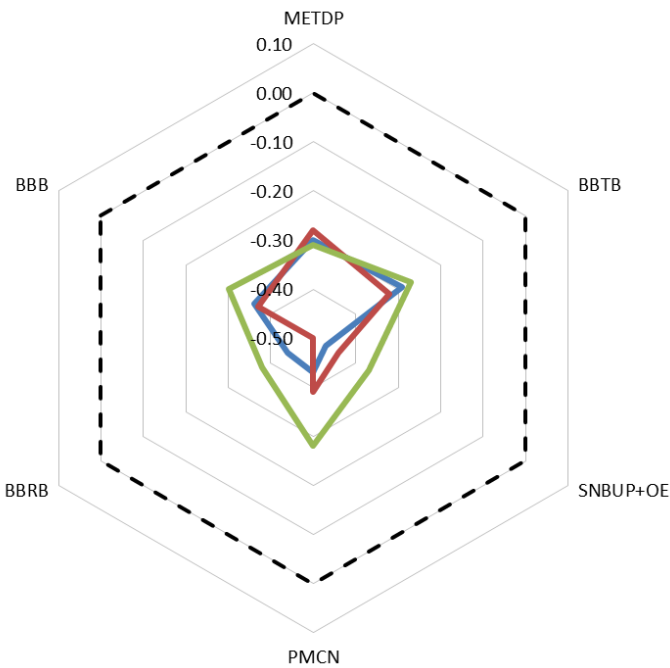
2018

Número de términos

Número de coocurrencias

Mundo 344.896; Alemania 49.527; Francia 35.446 ; España 29.157

Mundo 3.160.799; Alemania 163.429; Francia 102.498 ; España 82.419



\*METDP=Microelectronics Engineering and Top-down Processes; SNBUP+OE= Synthesis of Nanomaterials and Bottom-up Processes + Optics and Electronics; PMCN= Physical and Mechanical Characteristics of Nanomaterials; BB=Biotechnology and Biomedicine; BBTB=BB:Therapeutic Biomedicine; BBB=BB:Biosensing; BBRB=BB:Regenerative Medicine

**Figura 7.** Promedio del Índice de Especialización Relativo de Palabras Clave (RSIk) por temáticas para Alemania (azul), Francia (rojo) y España (verde) con respecto al mundo. Valores para el número total de términos (izquierda) y para el número total de ocurrencias (derecha)

## Capítulo 6. Limitaciones

Como cualquier tesis, esta investigación no está exenta de limitaciones.

La primera limitación es la estrategia de búsqueda. Los dominios científicos sumamente dinámicos experimentan cambios constantes, dando lugar a nuevas teorías, leyes y técnicas aplicadas que conllevan el uso de terminología novel. Por consiguiente, la estrategia de búsqueda requiere una actualización constante mediante la agregación de nuevos términos y la revisión de los ya existentes.

La segunda limitación es el reducido número de países analizados en el estudio de caso del tercer artículo. No obstante, el enfoque metodológico propuesto es extrapolable a otros países y a nivel institucional.

La tercera limitación hace referencia al Índice de Actividad. Este indicador puede presentar algunos problemas debido a su estructura matemática. Los valores de este indicador, para un dominio científico determinado, pueden verse afectados por la actividad en producción científica de los demás países en otros campos del conocimiento, de manera que su cálculo requiere de continuas actualizaciones (Rousseau & Yang, 2012). De igual manera, la interpretación de los resultados de este índice en el ámbito de la política científica debe abordarse con cautela (Rousseau, 2018; Stare & Kejžar, 2014).

La cuarta limitación alude al uso de la muestra elegida para el diseño del cuestionario enviado a expertos. Dicha muestra contiene publicaciones, pero se podría haber considerado una muestra formada por revistas. En cualquier caso, para ambas muestras se deben tener en cuenta características determinantes de la encuesta en línea con la finalidad de garantizar una alta tasa de respuesta de los encuestados (Liu & Wronski, 2017; Galesic & Bosnjak, 2009; Ganassali, 2008; Holbrook et al., 2006).

## **Capítulo 7. Conclusiones generales**

En esta tesis se ha analizado la evolución de la estructura intelectual y cognitiva de la NST como disciplina y se ha trabajado en la comparación de distintas clasificaciones temáticas que han puesto de manifiesto la problemática que existe en las clasificaciones y, por extensión, en cualquier análisis que derive de su uso.

La primera publicación usa una metodología que permite localizar, identificar y visualizar los principales temas de investigación que caracterizan un dominio científico complejo y con fronteras difusas, como es NST, así como otros aspectos relativos a sus dinámicas. Dicha aproximación permite estudiar cómo se desarrolla un dominio científico y qué disciplinas confluyen en él a lo largo del tiempo, así como los temas emergentes.

Las palabras extraídas de los títulos y los resúmenes contribuyen a determinar los aspectos más representativos de la investigación de un dominio científico. Al ser palabras extraídas del lenguaje natural, favorecen el establecimiento de una terminología más actualizada y la consecuente identificación de las tendencias dentro del discurso científico del campo del conocimiento (Porter et al., 2019; Wang et al., 2019). Sin embargo, el uso del lenguaje natural presenta el inconveniente de la dispersión terminológica, pues son términos no normalizados. Por tanto, el uso de un lenguaje natural reduce la rigidez y falta de precisión de los lenguajes controlados, pero aumenta las dificultades en el tratamiento de los datos.

Dependiendo del periodo estudiado, los términos y sus relaciones varían. Existen relaciones con un gran peso y que muestran una gran cohesión en comparación con el resto, lo que denota la presencia de frentes de investigación consolidados. Sin embargo, aparecen otras relaciones con un peso menor, lo que indica la existencia de frentes de investigación emergentes, frentes en los que los científicos pierden interés o frentes que

han sido absorbidos por otros más consolidados, lo que facilita la identificación de su estructura disciplinaria (Luan & Porter, 2017).

La capacidad de predicción de temas emergentes o nichos de investigación, además de su visualización, puede ayudar a los académicos, investigadores y gestores de política científica a comprender la estructura disciplinaria y sus relaciones con otras áreas de investigación (Wang et al., 2019; Suominen et al., 2016; Porter & Youtie, 2009a). Asimismo, facilita a investigadores y gestores identificar focos de atención que puedan repercutir positivamente en sus objetivos y aunar esfuerzos en esa dirección (Rotolo et al., 2015). Por ende, el método sugerido puede extrapolarse a otros dominios científicos o temas de investigación específicos, además de adaptarse a otros niveles de agregación (macro, meso y micro) (Boyack et al., 2014).

La comparación de diferentes metodologías para la delimitación temática revela la dificultad implícita en este proceso, especialmente cuando se trata de dominios científicos emergentes y complejos. Este hándicap pone de manifiesto la necesidad de elaborar arquetipos para refinar la delimitación de dominios y la necesidad de combinar y explorar distintas aproximaciones metodológicas. Además, hay que tener en cuenta que uno de los factores que afectan a la delimitación temática es el uso de determinadas fuentes de información (Strotmann et al., 2009) por los sesgos de temáticas o de representatividad de territorios en algunas bases de datos (Guerrero-Bote et al., 2021; Mongeon & Paul-Hus, 2016).

Más interesante aún son los resultados que muestran la opinión de los expertos en el proceso de delimitación. Su falta de acuerdo a la hora de asignar la integración o no de la literatura científica en NST viene condicionada por la especialidad temática a la que pertenecen. Si bien la validación de los resultados por parte de los expertos mejora la calidad del proceso de delimitación (Zitt et al., 2019; Zitt, 2015), el trabajar en determinadas líneas de investigación puede inclinar los resultados en favor

de algunas temáticas, provocando disparidades significativas que ponen de manifiesto que la perspectiva cualitativa tiene un fuerte componente de subjetividad. Por tanto, la opinión de los expertos debe ser abordada con cautela y utilizarse como complemento a otras fases en el cometido de la delimitación, y viceversa. Este hecho revela la necesidad de complementar análisis cuantitativos, con un carácter objetivo, con la opinión de los expertos que implica subjetividad.

Todo ello corrobora que son necesarios distintos enfoques y metodologías en la delimitación de dominios científicos (Colavizza et al., 2021), ya que inciden directamente en la fiabilidad y representatividad de la investigación. Su uso en la gestión de la investigación puede introducir distorsiones en los procesos de financiación (Abramo et al., 2019) o en la evaluación de la investigación (Gómez-Núñez et al., 2016), donde es necesaria una delimitación fiable de los campos del conocimiento.

El enfoque adoptado en la tercera publicación identifica la especialización temática de NST a nivel nacional en el panorama internacional. Los mapas solapados de copalabras a nivel global y entre países (Klavans & Boyack, 2011) identifican clústeres y tendencias recientes con bastante coherencia, mientras que el indicador de la especialización, aplicado a los términos, explora a fondo los diferentes clústeres y su terminología en un contexto global.

La premisa aquí fue explorar qué clústeres y términos presentaban una mayor especialización y si esta especialización se podría utilizar como ventaja competitiva a nivel de países. Los resultados muestran que los indicadores de especialización basados en datos de producción ayudan a identificar aquellas temáticas en las que los países parecen tener cierta ventaja competitiva con respecto a otros países. En este sentido, mientras que algunos países experimentan un rápido crecimiento en el número de publicaciones, el grado de especialización desciende. En cambio, hay países

que, sin ser los más productivos en términos de publicaciones, están enfocando su investigación en un área con mayor intensidad que otros. Esta observación evidencia que los perfiles de especialización en la investigación en NST pueden ser altos a pesar de una participación mundial relativamente baja.

El Índice de Especialización basado en Palabras se ha mostrado efectivo en la detección de términos que muestran una “ventaja competitiva”, identificando fortalezas propias y especialización internacional (Abramo et al., 2017; Hidalgo et al., 2007). Asimismo, el estudio de la evolución temporal del indicador resulta útil para la actualización de posibles áreas en las que especializarse y/o diversificarse a través de la detección de activos.

A la hora de establecer las prioridades en inversión, diagnosticar las áreas relevantes, identificando las fortalezas y las debilidades de un país dentro de un campo de conocimiento, puede ser una estrategia eficaz para el desarrollo de sus capacidades científicas. Tal diagnóstico fomenta la transformación positiva, avanzando en nuevas líneas de interés, actualizando áreas desatendidas o fortaleciendo aquellas que ya son competitivas a nivel internacional. Esta información resulta de utilidad para complementar las acciones encaminadas a la definición de líneas prioritarias en el diseño de estrategias de especialización inteligente, a través de los sistemas nacionales de investigación para el fomento y desarrollo de áreas emergentes o de tecnologías y aplicaciones novedosas (Youtie et al., 2021). Por tanto, estos resultados tienen implicaciones importantes en la política científica, ya que apuntan a los temas en los que un país podría promover esfuerzos de transformación y ganar ventaja competitiva dentro de un campo científico, así como fomentar colaboraciones y aumentar alianzas con otros países.

## Capítulo 8. Investigaciones futuras

Las futuras vías de investigación abarcan la extrapolación de la metodología propuestas en esta tesis a otras bases de datos de producción científica de carácter multidisciplinar, como, por ejemplo, Dimensions<sup>18</sup> y OpenAlex<sup>19</sup>. De igual manera, se plantea explorar y combinar aproximaciones, como la Altmetría, para analizar otras dimensiones en las que la producción científica tiene un impacto que no está exclusivamente restringido a la comunidad científica (Arroyo-Machado et al., 2022).

En relación con la especialización temática, la metodología descrita podría aplicarse en diferentes niveles de agregación macro y meso, y extender los análisis teniendo en cuenta las relaciones con la industria, para estudiar y comparar potenciales ventajas competitivas en cada uno de los niveles de análisis.

Otra posible e interesante línea de trabajo sería generar taxonomías de manera automática, que contribuyan a la actualización, mantenimiento y clasificación de la investigación en NST. Taxonomías que contemplasen todos los cambios que se produzcan dentro del dominio científico de manera clara y coherente a partir de técnicas de inteligencia artificial.

También se plantea explorar la transferencia de conocimiento de la producción científica al sistema productivo, permitiendo detectar el conocimiento científico útil para la generación de productos y servicios. Mediante el análisis de las citas que reciben los artículos científicos en las patentes de NST se podría determinar dicha transferencia. El estudio conjunto de producción científica y patentes puede dar lugar al desarrollo de un sistema híbrido (Jürgens & Herrero-Solana, 2017; Jürgens, 2016).

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<sup>18</sup> <https://www.dimensions.ai/>

<sup>19</sup> <https://docs.openalex.org/>



## **General conclusions**

In this thesis, we have analyzed the evolution of the intellectual and cognitive structure of the NST as a discipline and have worked on the comparison of different field classifications that delineated the scientific domain. These both have revealed the problems that exist in the classifications and, by extension, in any analysis that derives from its usage.

The first publication utilizes a methodology that allows locating, identifying and visualizing the main research topics that characterize a complex scientific domain with fuzzy borders, such as NST, as well as other aspects related to its dynamics. This approach allows us to study how a scientific domain develops and what disciplines converge in it over time, as well as the emerging topics.

The words extracted from titles and abstracts contribute to determine the most representative aspects of the research of a scientific domain. To be word extracted from natural language, they favor the establishment of a more updated terminology and the consequent identification of trends within the scientific discourse of the knowledge field (Porter et al., 2019; Wang et al., 2019). However, the use of natural language has the drawback of terminological dispersion, since they are non-standard terms. Therefore, the use of a natural language reduces the rigidity and lack of precision of controlled languages, but increases the difficulties in data processing.

Depending on the period studied, the terms and their relationships vary. There are relationships with a great weight and they show a great cohesion compared to others, which denotes the presence of consolidated research fronts. However, other relationships appear with a lower weight, which indicates the existence of emerging research fronts, fronts in which scientists loose interest or fronts that have been absorbed by more consolidated ones,

that facilitate the identification of its disciplinary structure (Luan & Porter, 2017).

The predictive ability of emerging topics or research niches, in addition to its visualization, can help academics, researchers and science policy managers to understand its disciplinary structure and its relationships with other research areas (Wang et al., 2019; Suominen et al., 2016; Porter & Youtie, 2009a). Likewise, it makes it easier for researchers and managers to identify focuses of attention that can have a positive impact on their objectives and to join forces in that direction (Rotolo et al., 2015). Therefore, the suggested method can be extrapolated to other scientific domains or specific research topics, in addition to being adapted to other aggregation levels (macro, meso and micro) (Boyack et al., 2014).

The different methodologies comparison for delineating fields reveals the implicit difficulty in this process, above all when it comes to emerging and complex scientific domains. This handicap highlights the need to develop archetypes to refine the field delineation and the need to combine and explore different methodological approaches. It should also be taken into consideration that one of the factors that affect the field delineation is the use of certain information sources (Strotmann et al., 2009) due to the biases of thematic or representativeness of territories within some databases (Mongeon & Paul-Hus, 2016).

Even more interesting are the results that show the opinions of the experts in conducting delineation. Their lack of agreement when assigning the integration or not of the scientific literature in NST is influenced by the topic specialty to which they belong. While validation of results by experts improves the quality of delineation process (Zitt et al., 2019; Zitt, 2015), to work on certain research fronts can tilt the results in favor of some topics, causing significant disparities which show that the qualitative perspective has a strong component of subjectivity. Therefore, the experts' opinion should approach

with caution and be used as a complement to other stages in the delineation task, and vice versa. This fact reveals the need for complementary quantitative analyses, with an objective character, with the experts' opinion that implies subjectivity.

All this verifies that different approaches and methodologies are needed for scientific domain delineation (Colavizza et al., 2021), since they directly affect the reliability and representativeness of the research. Their use in research management can introduce distortions in funding processes (Abramo et al., 2019) or in research evaluation (Gómez-Núñez et al., 2016), where a reliable field delineation is needed.

The approach taken in the third publication identifies the NST topic specialization at the national level on the international scene. The global overlay co-word maps and across countries (Klavans & Boyack, 2011) identify recent clusters and trends quite consistently, while the bibliometric indicator of specialization, applied to terms, thoroughly explores the different clusters and their terminology in a global context.

The premise here was to explore which clusters and terms had greater specialization and whether this specialization could be used as a competitive advantage at country level. The results show that specialization indicators, based on production data, help to identify those topics in which countries seem to have some competitive advantage over other countries. In this sense, while some countries experience a rapid growth in the number of publications, the degree of specialization decreases. Instead, there are countries that, without being the most productive in terms of publications, are focusing their research in one area with greater intensity than others are. This observation highlights that the specialization profiles in NST research can rise despite a relatively slight global participation.

The Relative Specialization Index based on keywords has been shown to be effective in detecting terms that show a great "competitive advantage",

identifying its own strengths and international specialization (Abramo et al., 2017; Hidalgo et al., 2007). In addition, the study of the temporal evolution of the indicator is useful for updating possible areas in which to specialize and/or diversify through the detection of assets.

When establishing investment priorities, diagnosing the relevant areas, identifying the strengths and weaknesses of a country within a knowledge field, can be an effective strategy to develop its scientific capabilities. Such diagnosis encourages positive transformation, advancing in new lines of interest, updating neglected areas or strengthening those that are already internationally competitive. This information is useful to complement the actions aimed at defining priority lines in the design of smart specialization strategies, through national research systems for the promotion and development of emerging areas or new technologies and applications (Youtie et al., 2021). Therefore, these results have important implications for science policy, since they point to the issues in which a country could promote transformation efforts and gain competitive advantage within a scientific field, as well as foster collaborations and increase alliances with other countries.

## Future research

Future avenues for research include the extrapolation of the methodology proposed in this dissertation to other traditional databases of scientific output, such as other multidisciplinary scientific output databases, such as Dimensions<sup>20</sup> y OpenAlex<sup>21</sup>. Likewise, it would be interesting to explore and combine other approaches, such as Altmetrics, so as to analyze other dimensions in which scientific output has an impact that is not exclusively restricted to the scientific community (Arroyo-Machado et al., 2022).

In relation to topic specialization, the methodology outlined in this research could apply at different macro and meso aggregation levels, and extend scientific analysis taking into account the relationships with the industry, in order to study and compare potential competitive advantages in each of the analysis levels.

Another possible and promising study would be to generate taxonomies automatically that contribute to updating, maintaining and classifying NST research. These taxonomies would track changes that take place within the scientific domain in a clear and coherent way from artificial intelligence techniques.

It is also needed to explore the knowledge transfer from research production to the production system, allowing the detection of useful scientific knowledge for the development of products and services. By analyzing the citations received by scientific articles in NST patents, such transfer could be determined. The joint study of scientific output and patents can lead to the development of a hybrid system (Jürgens & Herrero-Solana, 2017; Jürgens, 2016).

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<sup>20</sup> <https://www.dimensions.ai/>

<sup>21</sup> <https://docs.openalex.org/>

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## Parte II. Estudios empíricos

### Capítulo 9. Identification and visualization of the intellectual structure and main research lines in Nanoscience and Nanotechnology at the worldwide level

This chapter is published as:

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#### Abstract

The aim of this paper is to make manifest the intellectual and cognitive structure of nanoscience and nanotechnology (NST) by means of visualization techniques. To this end, we used data from the Web of Science (WoS), delimiting the data to the category NST during the period of 2000–2013, retrieving a total of 198,275 documents. Through direct author citation of these works, we identified their origins and the seminal papers, and through word co-occurrence extracted from the titles and abstracts, the main lines of research were identified. In view of both structures, we may affirm that NST is a young scientific discipline in constant expansion, needing time to establish its foundations but showing a strongly interdisciplinary character; its development is furthermore dependent upon knowledge from other disciplines, such as physics, chemistry, or material sciences. We believe that this information may be very useful for the NST scientific community, as it reflects a large-scale analysis of the research lines of NST and how research has changed over time in the diverse areas of NST. This study is moreover intended to offer a useful tool for the NST scientific community, revealing at a glance the main research lines and landmark papers. Finally, the methodology used in this study can be replicated in any other field of science to explore its intellectual and cognitive structure.

## 1. Introduction

Nanoscience and nanotechnology (NST) comprise the study, design, creation, synthesis, manipulation, and application of materials, devices, and functional systems by means of the control of the material at the nanoscale, as well as the exploitation of phenomena and properties of material at the nanoscale. It is a discipline that appears in the second half of the twentieth century, when Richard P. Feynman (1960) referred to the possibilities offered by the manipulation of material at the atomic scale. The discovery of the scanning tunneling microscope (Binnig and Rohrer 1983) in the 1980s opened the gates to the development of NST, as it allowed the scientific community to obtain new materials and minute machinery.

According to the literature, only in the past decade has NST taken off on an exponential voyage due to the advancements it holds for industry, health, the environment, and national security (Huang et al. 2011). Yet, negative social and environmental implications have also come to light, as well as a lack of knowledge about the risks that many of its applications could entail (Seaton and Donaldson 2005).

Many are the works that have studied the scientific literature in NST. For example, the study run by Braun et al. (1997) established a clearly exponential growth of the NST scientific output that started in the early 1990s on the basis of a dataset with the prefix nano in the title of science and technological journal papers (4152 papers) from Science Citation Index (ISI) in the period of 1986–1995. A year later, Meyer and Persson (1998) characterized nanotechnology showing its interdisciplinary nature. Using the same approach as Braun et al. (1997), they determined that the major rate growth of nano-paper is in natural and multidisciplinary science, while the field of engineering and material and life science would be less important in view of their negative rate of growth. The growth of NST has been registered both as scientific publications and as patents. Hence, the bibliometric perspective is ideal for observing scientific activity in this discipline, with its interdisciplinary



and multidisciplinary characters (Schummer 2004) and its widespread economic and social implications.

Kostoff et al. (2006b) appraised the growth of the nanotechnology research literature in the Science Citation Index, from 4552 articles in 1991 to 33,060 articles in 2004, and another study pointed out that “Global nanotechnology research article production has exhibited exponential growth for more than a decade”. They studied more than 65,000 records related to NST in the Science Citation Index/Social Science Citation Index (SCI/SSCI) in 2005 (Kostoff et al. 2007b). Porter et al. (2008) displayed the nano research publication activity from 1990 to 2006 from the Science Citation Index, finding growth in the nano research activity to be higher from the year 2000 onward. The number of papers in NST contained in WoS journals shows a steady increase since 2000 (Chen et al. 2013). Another study concludes that the number of nanotechnology journals has been growing steadily since the late 1990s (Grieneisen 2010). Such growth is also reflected in the Scopus database, where the documents published show a nearly threefold growth of NST world share output. The main growth spurt is between 2007 and 2013, a period when its world share output practically doubled (Chinchilla-Rodríguez et al. 2016a).

Beyond matters of growth, in recent years, many researchers have conducted scientometric analysis to define nanotechnology and capture its scope by using lexical queries (Porter et al. 2008; Huang et al. 2011; Grieneisen and Zhang 2011; Arora et al. 2013, 2014); to identify all disciplines that NST encompasses exhibiting the interdisciplinarity of NST (Porter and Youtie 2009); to explore the interdisciplinary characteristics of NST and investigate its intellectual structure (Jo et al. 2016); to give a global overview of the infrastructure of the global nanotechnology literature through most cited authors, journal, and papers, and prolific authors, journal institutions, and countries (Kostoff et al. 2006b); to study the network of citation in nanotechnology for patents, institutions, countries, and technology fields (Li et

al. 2007); to identify the core papers in NST and describe its genealogy (Kostoff et al. 2006a); to examine the cognitive structure, multidisciplinary, and evolution of NST (Milojević 2012); or to examine the research paper and patents involved in the coming generation of active nanotechnologies to delineate phases and possible emerging research directions (Suominen et al. 2016).

In addition, bibliometric techniques have helped to study the development of certain subfields or subjects within NST, for instance carbon nanotubes (Munoz-Sandoval 2014), carbon nanostructures (Terekhov 2015), nanoparticle generation by laser ablation in liquids (Barcikowski et al. 2009), nanotoxicology (Ostrowski et al. 2009), nano-energy (Menéndez-Manjón et al. 2011; Guan and Liu 2014), or microelectromechanical systems (MENS) (Hu and Liu 2015).

Other works have applied bibliometric techniques to analyze the evolution and position of NST in the international context, so as to gauge the scientific performance of countries (Chen et al. 2013; Chinchilla-Rodríguez et al. 2016a); to compare developed and developing countries (Jafari and Zarghami 2016); to highlight activity and visibility in the global landscape of some countries, among them Russia (Terekhov 2012) or the Siberian Branch of the Russian Academy of Science (Lavrik et al. 2015), in Latin America (Invernizzi et al. 2015; Chinchilla-Rodríguez et al. 2016b), in Mexico (Lau et al. 2014), in Venezuela (López Cadenas et al. 2011), or Pakistan (Bajwa and Yaldram 2012); to evaluate the productivity, dominant research topics, and diffusion patterns in Russia, China, and India using papers from WoS and patents from US Patent and Trademark Office (USPTO) (Liu et al. 2009); to identify the risky nanomaterials that the nano-environmental, health, and safety community might examine through study of patent literature from USPTO and World Intellectual Property Organization (WIPO) and the Project on Emerging Nanotechnologies consumer product database (Leitch et al. 2012); or to identify growth trends, research topics, and the evolution in National Science

Foundation (NSF) funding and commercial patenting activities at USPTO (Huang et al. 2006).

Among the array of bibliometric techniques available today, science mapping is particularly useful for analyzing and visualizing the social and intellectual structure or dynamics of scientific research fronts (Braam et al. 1991a, b; Noyons et al. 1999; Börner et al. 2003). These representations, dating back to the seventies, allow users to explore relationships involving the selected unit of analysis (Small 1973; Small and Griffith 1974; Small and Sweeney 1985; Small et al. 1985). In the 1980s, they underwent a controversial period of development and virtual brainstorming to confirm their validity (Leydesdorff 1987; Hicks 1987; Tijssen et al. 1987). This led to a slowdown in the absorption of scientific policy in the 1990s, when more user-friendly interfaces became commonplace. In the past 10 years, their use has been extended and their utility is a matter of consensus, due largely to the greater availability of data, with important expert contributions in the field of computation specializing in information visualization (Börner et al. 2003). Today's science maps have benefited from a combination of new algorithms, the enhanced potency of calculation, and the robustness of results, as one can generate and guarantee a stable template at the worldwide level to be used as the basis for analysis (Moya-Anegón et al. 2004, 2007; Boyack et al. 2005; Leydesdorff and Rafols 2009; Rafols et al. 2010).

The development of techniques such as overlay maps (Rafols et al. 2010) makes it possible to generate such stable templates of scientific maps at the global level, for their later use to compare aspects of an organization, a field of research or the scientific output contained in databases such as the Web of Science (Thomson Corporation 2015b) or Scopus (Elsevier 2015). The cognitive structure of a scientific domain may thereby be analyzed in a geographic sense, or to perceive its evolution and the emerging lines of research that may be a priority for the economic policy of a government (Leydesdorff and Rafols 2011; Leydesdorff et al. 2015).

Such maps can thereafter serve as units of analysis regarding authors, documents, journals, or relevant term/words. Authorship is used to trace the social and intellectual structure (scientific paradigm) of a discipline, field, or specialty (Chen 1999; Garfield et al. 2003). Documents are used to visualize a knowledge domain or to assess research (Small 1999; Noyons et al. 1999). Journals can project a macro view of science or differentiation in a discipline (Leydesdorff 1987; Boyack et al. 2009).

Direct citation networks are considered the most efficient means of exploring how the scientific paradigm of a discipline is built through its own history and development (Garfield et al. 2003; Garfield 2004, 2009). Garfield points out that the most relevant nodes shown in a network constitute a landmark event in the broader development of a knowledge domain.

Although bibliometric techniques use citation analysis to study the yield of a discipline in terms of the impact or strength of influence of research efforts, using citation in the present work has nothing to do with the use (or misuse) of the journal impact factor for the promotion and financing of authors. We do not attempt to analyze the quality of research; citation is merely used to follow the flow of ideas and knowledge recorded as references made by authors when they root or support their ideas in background papers (Narin 1976; Garfield 1979). Mention of a document is a means of manifesting the relationship between a citing work and the cited work at a particular point in the development of research (Sandison 1989; Egghe and Rousseau 1990).

Our perspective with this understanding of citation focuses on identifying research topics or disciplines in cognitive networks and uncovering the intellectual structure of a discipline by the use of direct citation networks where each node represents a piece of knowledge and each link denotes the knowledge flow (Newman 2003). The analysis of citation networks, from a scientometric perspective, can help identify core literature (Potter 1988), retrace the diffusion of ideas or trace the structure of knowledge (Soper et al.

1990), or look at communication patterns, identifying the most influential authors and papers (Lawani 1980). The interpretations brought out through citation analysis applied to books and journals of a specific discipline can also testify as to its historical movement and determinant production at the national or international level (Lawani 1981).

The use of journal articles—adopted in this work as a single evaluation unit—is based on the notion that journal literature is the most formal channel of communication for scientists (Bellardo 1980) and lies at the heart of scientific and technical communication (Tomajko and Drake 1985), allowing the dissemination of information across geographical borders by scientists in any field of knowledge (Borgman 1989). In no case were journals from WoS used to quantify impact. This journal set was selected because WoS provides mature, reliable source material for mapping science (Leydesdorff et al. 2010).

Co-word analysis is a means of studying the association between the most representative terms of scientific literature, likewise lending the opportunity to obtain further information about the underlying structure and the overt tendencies of a given scientific discipline (Ding et al. 2001; Cantos-Mateos et al. 2012). Words themselves lead us to familiarity with living science and have the capacity to reflect scientific, social, and political contents that pertain to the most controversial domains or least understood emerging areas (Cantos-Mateos et al. 2014). The combination of frequency of appearance of terms, together with the techniques of spatial representation based on multidimensional scaling (MDS), provides us with information about the main research topics or those that prevail over a given period of time.

We can trace co-word analysis back to the 1980s (Callon et al. 1983; Leydesdorff 1989), when it was described as the best method to know and explain the cognitive structure of a field at the level of research specialties (Small and Griffith 1974; Braam et al. 1991a, b), moreover capable of

revealing new developments of a field over time (Peters and van Raan 1993). This type of analysis was applied to polymer chemistry (Callon et al. 1991), to neural network investigation (Van Raan and Tijseen 1993), to information retrieval (Ding et al. 2001), to Information Sciences (Van Den Besselaar and Heimeriks 2006), to the links between opportunistic infections (IOs) and HIV/AIDS (Onyancha and Ocholla 2005), to the Economy (Cahlík and Jiřina 2006), to secure information (Lee 2008), Ecology (Neff and Corley 2009), to biodiversity and conservation (Liu et al. 2011), or to corporate social responsibility (Qin et al. 2016), among others.

It is assumed that NST is an attractive new scientific discipline, in which many researchers, countries, and institutions want to be involved. Its study by the use of different bibliometric, scientometric, or informetric methodologies stands as a sign of the interest that NST holds in the worldwide R&D context given the many economic benefits for developed and developing countries (Wood et al. 2003) with their variety of impending needs (Beumer 2016).

Our hypothesis stems from the premise that the bibliographic references cited in research papers are an indicator of the influence that they have on the scientific community, conditioning scientific progress and provoking new ideas and subject areas; co-word analysis furthermore marks changes in the different research lines that make up a discipline. Accordingly, our study has a triple objective. Firstly, it aims to detect the origin of and trace the evolution of the intellectual structure of NST by means of the analysis of direct citation of works. Secondly, it attempts to identify and analyze the cognitive structure over time (active research lines) by means of co-word maps to exhibit changes taking place in NST. Thirdly, the methodology described offers another perspective of NST as a discipline by means of citation and co-word analysis.

## 2. Materials and methods

The Web of Science (WoS) was the database utilized to retrieve the set of documents on NST. Up to the time when this study was undertaken, it was the only multidisciplinary and international database containing this category, created in 2005, and composed following the Journal Citation Report (JCR) (Thomson Corporation 2015a) Science Edition 2014 by 73 journals. This source was the foundation of our search strategy. An abbreviated journal title query was subsequently designed and entered into the WoS database search engine for the version Science Citation Index Expanded 2014 (Appendix A).

Evidently, the NST category in WoS does not cover all the journals that publish articles about NST. It includes only the best journals. For this reason, we decided to design our search strategy using the JCR journals in the NST category, as the top journals of a discipline can be viewed as a sound tool for scientific evaluation (Garfield 1972, 1980). Although the number of NST journals has shown steady growth since the late 1990s, many articles about NST are also published in multidisciplinary science journals such as *Science* or *Nature*, or in highly specific discipline journals such as *Angewandte Chemie* or *Applied Physics Letters* (Grieneisen 2010). This is because many NST research lines in NST are not yet mature—still in the launching stage. As we needed to choose the journal set that would best represent NST as a discipline, we looked to JCR, whose journals might contain references to articles published elsewhere, that is, not exclusively in specialized NST journals.

Our search strategy used the field Publication Name, as this field is less problematic than others; it can retrieve more than 100,000 documents when combined with other fields (Arencibia-Jorge et al. 2009), yet in this case, it was limited by the time frame of study.

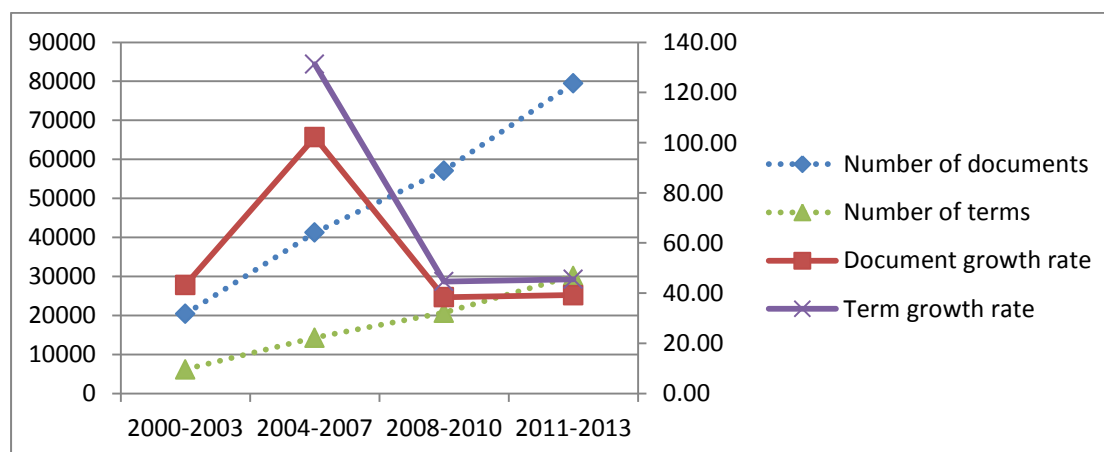
The period 2000–2013 was selected based on the papers of Grieneisen and Zhang (2011), who state that since 1998, nanoscale studies have grown in

alarming proportions in the entire body of research. In addition, the choice of a short time period allows for the published documents to play on an equal level with the documents published previously, which may have received numerous citations; in short time periods, the documents involved are all recent and have not yet generated substantial citation (Kostoff et al. 2008). Subsequently, we chose 2013 as the last year for the sampling time frame.

The discovery of graphene in 2004, the design of new programs and software like Gaussian (2003 or 2009) or SIESTA in 2002, the use of nanowire for solar cells or as nanosensors for the detection of biological and chemical species in 2001, the characterization of gold nanoparticles in 2004, etc., these are only a few examples of core papers in NST published in the first decade of this century.

In June of 2015, we launched our search into the WoS database search engine. The number of retrieved documents ([Figure 1](#)) from 2000 to 2013 was 198,275 and includes the following types: articles (187,949), proceedings (26,606), reviews (4066), editorial materials (3116), new items (1378), corrections (1223), letters (386), biographical items (80), meeting abstracts (70), book chapters (6), bibliographies (5), and reprints (2).

**Figure 1.** NST retrieved documents from WoS and relevant terms





## 2.1. Intellectual structure and detection of seminal papers

Citation-Assisted Background (CAB) (Kostoff and Shlesinger 2005) was used to identify seminal papers. CAB is based upon the assumption that seminal documents tend to be highly cited by the active researchers who belong to a specific scientific discipline; hence, any reference to these seminal documents will tend to be positive (Kostoff and Shlesinger 2005; Kostoff et al. 2006a). A file was generated where all downloaded documents were combined and a citation analysis was performed to identify the most cited documents of the dataset, using CitNetExplorer (Van Eck and Waltman 2014b), for visualizing and analyzing citation networks of scientific publications. This tool was used to create and visualize the intellectual network. The uncovered network featured a static structure that relied on papers as units of analysis and citations as units of measure.

The values applied to visualize information must range between 25 and 125 (White 2003). In our case, a total of 80 most-cited papers was the cutoff established, because a higher number of nodes would show too many relationships, and the viewer would perceive excessive information and an overlap of labels. This problem is known as an incomprehensible “clutter of links”.

After identifying the 80 most cited documents, we downloaded the most-cited documents which were not included in the initial dataset for one of two reasons: (a) either the documents had been published in journals that did not belong to the category of JCR NST or (b) the documents had been published before the year 2000. To download these most-cited documents from WoS, we executed different searches in the Title field, i.e., each most-cited title paper was tracked down in the Title field in WoS. This proved to be a crucial step in the process of generating the network using CitNetExplorer software. Otherwise, the nodes would have appeared as isolated nodes instead of as related nodes.

After this process, all the new downloaded papers were input into the initial dataset and a new citation analysis was performed, again using CitNetExplorer, showing the 80 most cited papers identified above and their relationships.

We should point out that downloading the most cited papers that were not included in the initial data set proved to be an essential step in our methodology, enabling us to explore the intellectual structure of NST and the relations between its nodes. If our network had only shown the most cited documents, no relationship with documents published before the year 2000 or with documents not published in JCR NST journals would have become apparent.

For the detection of the different clusters, CitNetExplorer applies an algorithm based on a variant of the modularity, by virtue of which the documents appear grouped in different clusters depending on the function of the distance in between them, so that the documents with a high degree of relatedness are found next to each other, and therefore form part of one same cluster (Van Eck and Waltman 2014a).

## 2.2. Cognitive structure

Co-word maps allow us to represent the cognitive structure of a discipline, identifying the research lines that form it and detecting future lines of research by means of clustering techniques (Callon et al. 1986; He 1999).

The detection of the main research lines and their evolution using longitudinal maps or networks reveals the best consolidated lines as well as the emergent ones. Used here as the unit of analysis were the words contained in the titles and the abstracts of the set of documents retrieved (Fig. 1); their co-occurrence as units of measurement; and, as the tool for the generation and visualization of the network, VOSviewer software (Van Eck et al. 2010; Van Eck and Waltman 2015).

In an effort to control the acronyms presented by many of the terms contained in the data file, we generated a thesaurus<sup>Footnote1</sup> with the most frequent acronyms. The second function of this thesaurus was to eliminate the terms of little significance contained in the documents. However, no thorough normalization of the data was carried out, which might have distorted the reality of our unit of analysis (words).

The number of words in each map increased steadily due to the rise in scientific production over the past decade. To avoid excessive noise and show only the most significant terms, a minimum occurrence threshold of 5 was established (a term was shown if it appeared at least five times). Furthermore, the VOSviewer default setting was used, meaning that 60% of the most relevant terms were displayed for each period. At any rate, a cluster should have at least ten words to be represented.

To detect the different clusters, the VOSviewer algorithm—an improved version of multidimensional scaling (MDS)—was used. This enabled us to avoid problems associated with MDS visualization such as generating circular representations or displaying the most relevant terms in the center of the representations (Van Eck and Waltman 2010).

The creation of a single map might entail some loss of information about changes in the main research lines of a discipline over time. In addition, because the number of documents per year has increased dramatically since 2000, new research trends have sprung up. With the utmost objective of representing the evolution of the cognitive structure of NST over time, without provoking a loss of structural information, we opted to make maps applying a temporary division into four sub-periods: longer periods (4 years) for the first temporal windows (2000–2003 and 2004–2007) and shorter ones for the following (3-year) periods (2008–2010 and 2011–2013) (Vargas-Quesada et al. 2010; Moya-Anegón et al. 2006). This basically resolved the problem related with the number of terms that made up each map, since the number of

documents that comprised scientific output in NST in 2000–2007 is inferior to the figure for 2008–2010. Therefore, the generation of maps covering the same number of years can be said to mask reality in the displays owing to this difference in the number of terms intervening.

Each one of the circles depicted in the maps makes reference to a term, its size being proportional to the number of co-occurrences with other terms. The proximity of some terms with others indicates the association or similarity existent among them, that is, the nearer two terms are to each other, the stronger their association. To the contrary, two terms far from each other point to a low level of mutual association. The color of the circles indicates belonging to a cluster, and every cluster or grouping, with its nodes, is therefore depicted in a different color.

### **3. Results and discussion**

The average growth of NST scientific output in the time frames established for creating our maps was 55.78%. However, the period of 2004–2007 showed an outstanding growth rate of 102.17%, followed by years 2000–2003 (43.32%), 2011–2013 (39.20%), and 2008–2010 (38.41%). As for the annual growth rate, 2007 is the most remarkable year, witnessing an increase of 41.24% in NST output, followed by 2006, with 25.02%, and 2003, with a growth rate of 24.74%.

Focusing on the evolution of the number of most relevant terms for each period again signals 2004–2007 as the window of greatest growth (131.11%), after which the figures remain quite stable, from 44.66 to 45.53%.

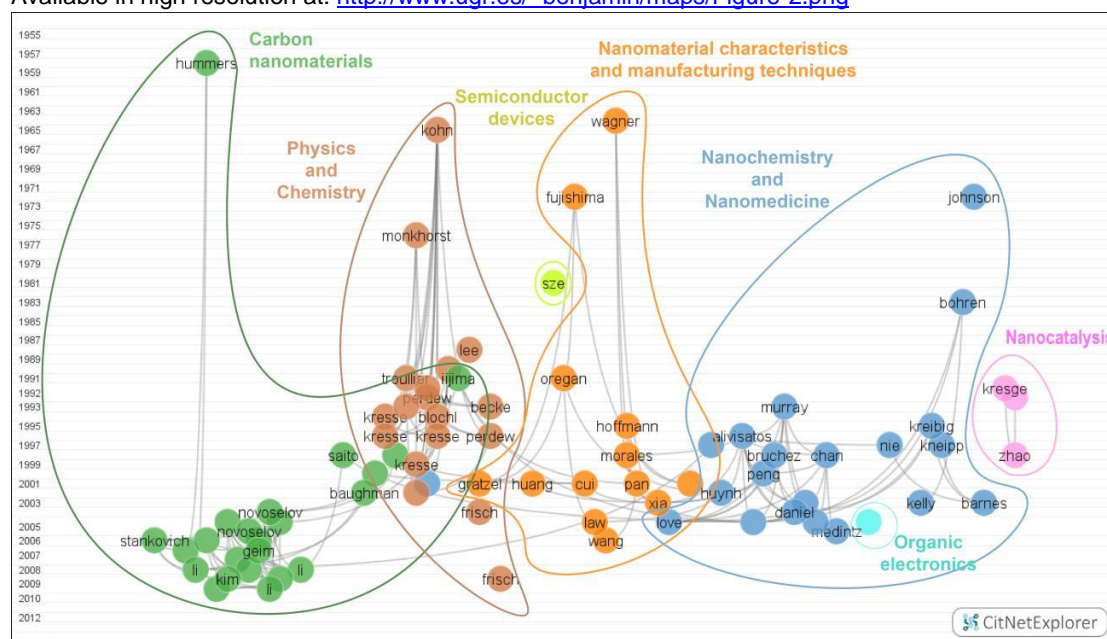
A comparison of the average growth in the number of documents and the number of terms reveals a peak in the first periods of study, followed by a relatively stable trend in later periods.

### 3.1. Intellectual structure NST–seminal papers

[Figure 2](#) shows the citation network with the 80 most-cited works throughout 2000–2013. The oldest of these papers detected goes back to 1958, and the most recent one is from 2009. Nodes of the citation network were cited at least 607 times from the dataset with 197,042 documents, leading to a sum total of 1,262,640 references. They appear in seven clusters that were studied selecting the Drill down option of CitNetExplorer, which offers an intuitive way of moving through the colored clusters. The maximum number of nodes in the clusters is 23 and the minimum is 1, because the nodes that form every cluster have been cited more than 607 times by the dataset.

**Figure 2.** The 80 most cited document network in NST

Available in high resolution at: <http://www.ugr.es/~benjamin/maps/Figure-2.png>



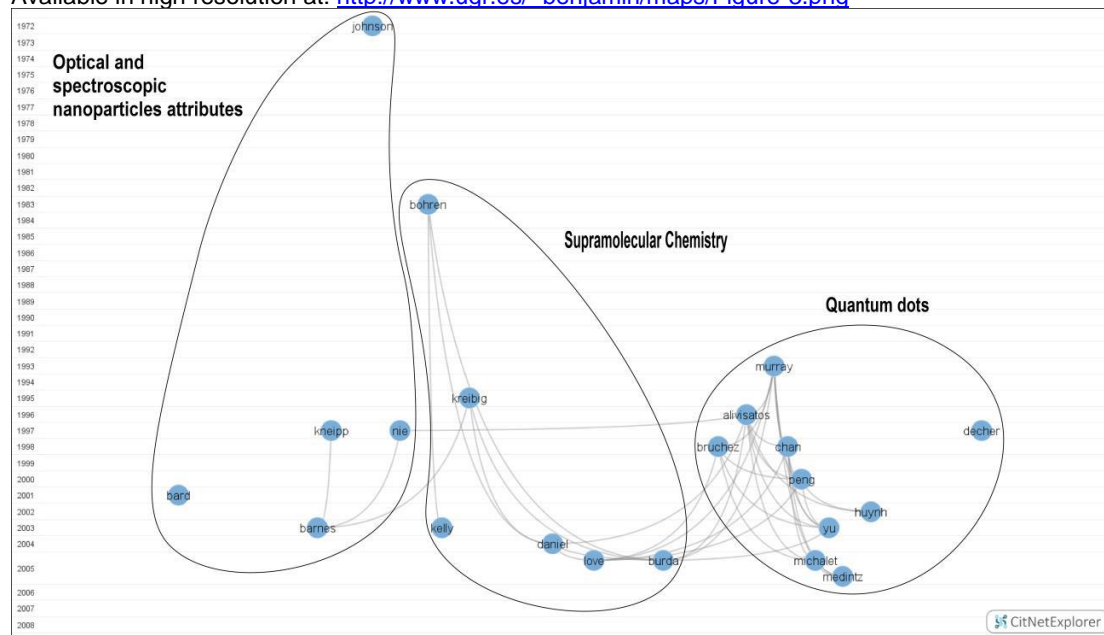
#### *Blue cluster: Nanochemistry and Nanomedicine (21 nodes)*

Inside this cluster ([Figure 3](#)), four different subgroups can be identified. To the right, we find papers by authors Murray et al. (1993), Alivisatos (1996), Decher (1997), Chan and Nie (1998), Bruchez et al. (1998), Peng et al. (2000), Huynh et al. (2002), Yu et al. (2003), Michalet et al. (2005), and Medintz et al. (2005). All of them concentrated their research activities on

Quantum dots: composition; shape; size; and spectroscopic, electronic, and thermodynamic attributes. Alivisatos' work is considered the most important in that area, bearing considerable influence on posterior research. In the middle are works related to Supramolecular chemistry. These papers were published by Bohren and Huffman (1983), Kreibig and Vollmer (1995), Kelly et al. (2003), Daniel and Astruc (2004), Love et al. (2005), and Burda et al. (2005). On the left appear papers about Optical and spectroscopic nanoparticle attributes. It is easy to see a major gap between the early work (Johnson and Christy 1972) and the subsequent development around 1997, when interest in this field peaked. All the areas of this cluster are seen to be associated with the research undertaken in Nanochemistry and Nanomedicine.

**Figure 3.** Nanochemistry and Nanomedicine

Available in high resolution at: <http://www.ugr.es/~benjamin/maps/Figure-3.png>

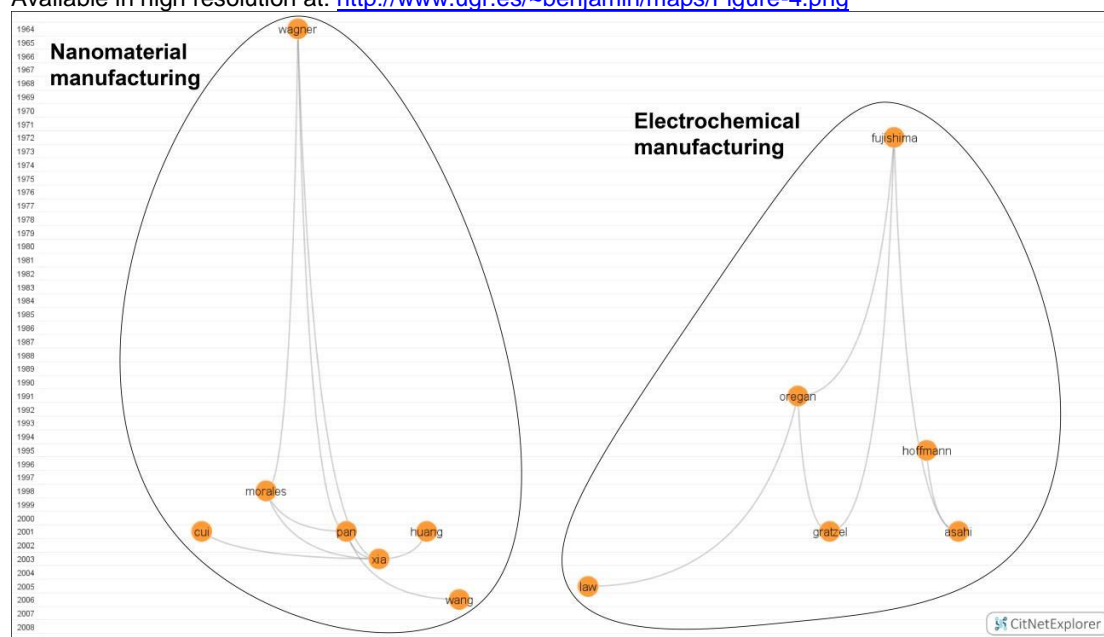


*Orange cluster: Nanomaterial characteristics and manufacturing techniques  
(13 nodes)*

Works of this cluster ([Figure 4](#)) are focused on the study of bottom-up nanomaterial manufacturing techniques, although we can divide the cluster into three sections. Papers on the right explore nanomaterial manufacturing, e.g. involving nanowires or nanobelts. Wagner and Ellis' work in 1964 was the forefather in this field. Afterward came works by Morales and Lieber (1998), Cui et al. (2001), Pan et al. (2001), Huang et al. (2001), Xia et al. (2003) and Wang and Song (2006), the latter cited because of his review of one-dimensional nanostructures.

On the other side of the map we find works about the manufacturing of devices to generate power energy or chemicals using electrochemistry techniques. Fujishima (1972) was the pioneer in this area, but it was not until 1991 when Oregan and Grätzel published a work that sorted out the problems suggested by Fujishima, using dye-sensitized colloidal titanium oxide to create efficient and economical solar cells (Oregan and Grätzel 1991). The papers by Hoffmann et al. (1995), Asahi et al. (2001) and Grätzel (2001) address environmental concerns through semiconductor catalysis, using solar irradiation or interior lighting to generate cheap and flexible photovoltaic cells based on nanocrystalline materials and conducting polymer films as a new generation of photoelectrochemical cells. Law's node appears a bit separate from the others because this paper used nanowires as solar cells to further increase their efficacy (Law et al. 2005).

**Figure 4.** Nanomaterial characteristics and manufacturing techniques  
 Available in high resolution at: <http://www.ugr.es/~benjamin/maps/Figure-4.png>



*Brown cluster: Physics and Theoretical chemistry (18 nodes)*

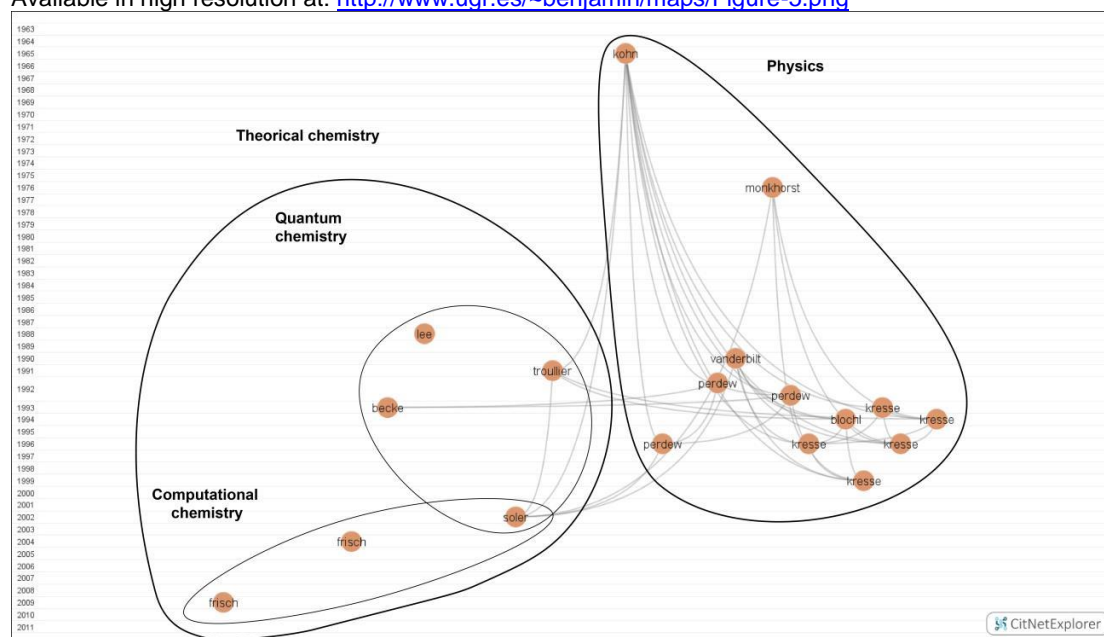
Here (Figure 5), we find the fundamental research in NST associated with Physics and Chemistry. Physics occupied the right side of the map, and Chemical Theory is on the left, in turn divided into two different groups: Quantum chemistry and Computational chemistry.

On the side of Physics, deserving mention is a work from 1965 presenting equations that solved the Density Functional Theory (DFT) (Kohn and Sham, 1965), whose theorem was published the previous year. However, this theory was modified in 1990 because of its imprecision, especially for chemical applications. Another contribution to DFT is the Perdew et al. paper (1996), the second most cited work in the citation network, about the exact exchange-correlation functional called Generalized Gradient Approximation (the first did not solve Kohn and Sham's equation). In addition, Lee et al. (1988) and Becke's (1993) works encouraged the exchange-correlation functional.



**Figure 5.** Physics and Chemistry

Available in high resolution at: <http://www.ugr.es/~benjamin/maps/Figure-5.png>



The Projector Augmented Wave method (PAW) was developed in order to calculate electronic structures through the pseudopotential method and linearized augmented planewave method (Blöchl 1994).

Kresse's works contributed to the development of essential principles (ab-initio) of DFT, combining different methods to quickly solve Kohn and Sham's equations (Kresse and Hafner 1993, 1994; Kresse and Furthmüller, 1996a, b; Kresse and Joubert, 1999). The percentage of citation of these key papers is very high, indeed comprising most of the highly cited works.

On the other side, the Quantum chemistry group contains 4 nodes. Papers by Troullier and Soler are represented on the right. The first explored pseudopotentials, with applications to some materials through plane wave calculations (Troullier and Martins 1991). Soler and colleagues' work designed a program called SIESTA (Spanish Initiative for Electronic Simulations with Thousands of Atoms) that combined DFT-related methods to calculate electronic structures and ab initio molecular dynamics (Soler et al. 2002). Slightly to the left appear Lee and Becke's works. Lee and colleagues developed a Colle-Salvetti correlation energy formula as a functional of the

electron-density (Lee et al. 1988), while Becke presented an improvement of the thermochemical Kohn-Sham density-functional theories with gradient corrections for exchange-correlations (Becke 1993).

The computational chemistry subgroup is located under the Quantum chemistry group. The different software versions of Gaussian (03 and 09) (Frisch et al. 2004, 2009) are displayed in this group. These programs have been used in NST to run a variety of electronic structure calculations and to predict molecular properties and chemical reactions. Soler's work also pertains to this group, as it proposed a computer program to implement SIESTA.

Most nodes here have been highly cited. Hence, it can be said that this is prestigious work presenting ideas or discoveries that proved essential for the development of NST, as it is impossible to study applied science without fundamental research.

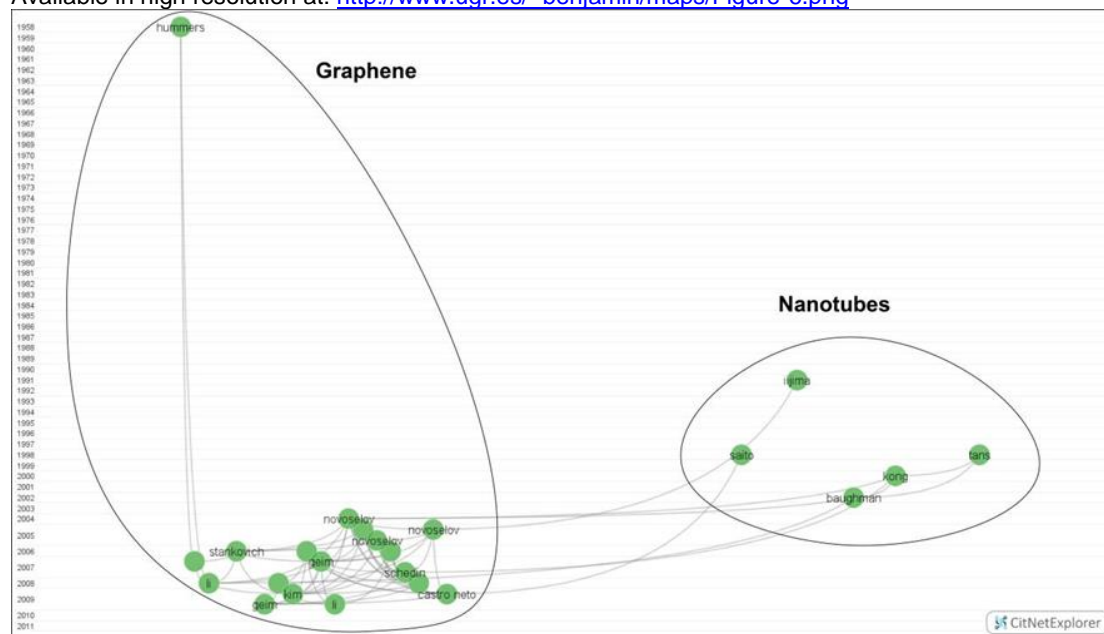
*Green cluster: Carbon nanomaterials (23 nodes)*

This cluster ([Figure 6](#)) reflects a current research boom: carbon nanomaterials, such as nanotubes or graphene. The first work was published by Hummers and Offeman (1959): graphite was synthesized in order to obtain graphite oxide. Several decades later came the landmark discovery of carbon nanotubes by Iijima (1991), which revolutionized NST and inspired prolific research by Tans, Verschueren and Dekker (1998), Kong et al. (2000), Baughman, Zakhidov and de Heer (2002) and so on. Nanotubes led to the development of graphene in 2004 by Novoselov et al. Nowadays, many basic and applied research efforts are focused on graphene —how to synthesize this nanomaterial, how to handle it without breaking or modifying it, or finding new applications according to its electronic, optic, thermal and mechanic characteristics. Hence, as the map shows, all nodes below the graphene node have dealt with this material.

A glance at the green cluster shows that many nodes have been cited in a short period of time. In other words, work with graphene tends to be highly cited. This new research line shows great promise for the future.

**Figure 6.** Carbon nanomaterials

Available in high resolution at: <http://www.ugr.es/~benjamin/maps/Figure-6.png>



*Pink cluster: Nanocatalysis (3 nodes)*

Works in this cluster ([Figure 2](#)) involve the synthesis of nanoporous materials and the application of mesoporous (pore size to 2 from 5nm) materials in the synthesis of chemical products, known as Nanocatalysis (Kresge et al. 1992; Beck et al. 1992; Zhao et al. 1998).

*Light blue cluster: Organic electronics (1 node)*

Research on producing photovoltaic power using polymer devices is displayed in this cluster ([Figure 2](#)). In particular, Li and colleagues' work studied photovoltaic polymer cells whose electric characteristics (conductivity) lend them to further applications (Li et al. 2005).

*Yellow cluster: Semiconductor devices (1 node)*

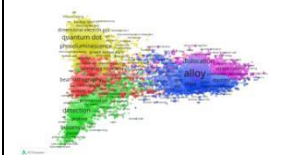
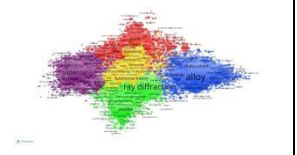
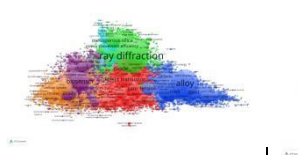
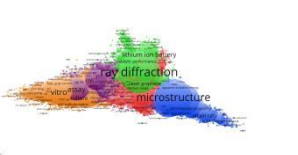
There is only one node in this cluster: Sze (1981). This work is held to be a main reference in the field of *semiconductor devices* (Figure 2).

### 3.2. Cognitive structure—research patterns and emerging trends

This section shows the evolution of NST research from 2000 to 2013 by means of science maps generated with VOSviewer. Tables 1 and 2 make it easy to schematically view the clusters identified, using the VOSviewer algorithm, in the different periods and their relationships with the rest of the clusters.

Tables 3, 4, 5 and 6, given below, present the 15 terms with the highest score (according to VOSviewer) for each cluster, and for each period studied. None of these 15 terms is repeated in other periods. Yet if we increase the cutoff to 30 or even to 50 terms, there are repetitions—even though the order of occurrence varies. This is an indication that the evolution of NST research is quite rapid, and the research lines tend to change as new advances are made.

**Table 1.** Science maps NST

aFigure 7. Science map NST 2000-2003 (6,189 items)	bFigure 8. Science map NST 2004-2007 (14,316 items)	cFigure 9. Science map NST 2008-2010 (20,709 items)	dFigure 10. Science map NST 2011-2013 (30,137 items)
			

aAvailable in high resolution at: <http://www.ugr.es/~benjamin/maps/N&N-2000-2003.png>

bAvailable in high resolution at: <http://www.ugr.es/~benjamin/maps/N&N-2004-2007.png>

cAvailable in high resolution at: <http://www.ugr.es/~benjamin/maps/N&N-2008-2010.png>

dAvailable in high resolution at: <http://www.ugr.es/~benjamin/maps/N&N-2011-2013.png>

**Table 2.** Identified clusters between 2000-2013

2000-2003	2004-2007	2008-2010	2011-2013
Microelectronics engineering and top-down processes	Microelectronics engineering and top-down processes	Microelectronics engineering and top-down processes	Microelectronics engineering and top-down processes + Organic electronics
Synthesis of nanomaterials and bottom-up processes + Biotechnology and Biomedicine	Synthesis of nanomaterials and bottom-up processes	Synthesis of nanomaterials and bottom-up processes + Optics and electronics	Synthesis of nanomaterials and bottom-up processes + Optics and electronics
Mechanical characteristics of materials	Mechanical characteristics of materials + Physical characteristics of materials	Mechanical characteristics of materials + Physical characteristics of materials	Mechanical characteristics of materials + Physical characteristics of materials
Optics and electronics	Optics and electronics	Biotechnology and Biomedicine: Biosensing	Biotechnology and Biomedicine: Biosensing
Physical characteristics of materials	Biotechnology and Biomedicine	Biotechnology and Biomedicine: Therapeutic biomedicine Organic electronics	Biotechnology and Biomedicine: Therapeutic biomedicine

*Optics and electronics (yellow cluster)*

In most of the maps this cluster occupied a central position, connected with the other clusters, a stem of sorts for the development of the NST network. Optics and electronics provide foundations for chemical applications and for biomedicine.

In the first period ([2000-2003](#)), *Optics and electronics* appears closely linked in its upper sector to *Microelectronics engineering and top-down processes*, and in its lower part to *Synthesis of nanomaterials and bottom-up processes*.

The following period ([2004-2007](#)) shows how this cluster begins to gain strength and influence in the rest of the research lines, with great relevance for *Synthesis* and *bottom-up processes*.

From [2008 to 2010](#), *Optics and electronics* is absorbed by the cluster *Synthesis of nanomaterials and bottom-up processes*, forming a single cluster. This union is due to the application of *bottom up* processes and

chemicals within *Optics and electronics*, for instance optic sensors. At the end of the second study period, in 2007, the application of optic sensors takes off, out of the laboratory and into applied science. After 2008 *Optics and electronics* is seen to approach the clusters *Synthesis of nanomaterials and bottom-up processes* and *Biotechnology and Biomedicine (Biosensing and Therapy)*. In 2007 optic devices began to be used in biotechnology and medicine. At the same time, the nature of the material underwent development, first with inorganic and then with organic materials. For this reason the term “quantum dot” disappears after 2008 and gives way to the entry of “graphene”.

The final period studied ([2011-2013](#)) continues to show a union of clusters *Optics and electronics* and *Synthesis of nanomaterials and bottom-up processes*, and suggests that these areas are bound to develop in tandem or even mutual dependence, eventually becoming one area.

#### *Synthesis of nanomaterials and bottom-up processes (green cluster)*

The cluster *Synthesis of nanomaterials and bottom-up processes* appears closely tied to the cluster *Optics and electronics* because in NST the bottom up materials are widely studied for optical applications. These are in turn used in sensors for biodetection and for the treatment of disease (biomedicine).

Like the cluster *Optics and electronics*, this one first involves inorganic materials, but then progresses toward the almost exclusive use of organic materials by 2009.

From [2000 to 2003](#), this cluster is fused to the cluster *Biotechnology and Biomedicine*. However, from [2004 to 2007](#) they separate, giving rise to two distinctive neighboring clusters. It was in this period when the nucleus of optic sensors underwent development. In the period [2008-2010](#) this cluster appears linked to *Optics and electronics*. Meanwhile, one sees that this cluster begins to interact with the cluster *Microelectronics engineering and top-down*

processes, and we begin to see terms indicating the real applications of the top-down nanomaterials (microfluid, microchip, micro channel). At the same time biosensors begin to be applied, namely in 2008. In 2009 biosensors were introduced in microfluid devices and there was an explosion of output in biomedicine... hence a new line of research appears. During the final interval of study ([2011-2013](#)) we find a new cluster next to this one, representing work with organic materials (*Organic electronics*).

**Table 3.** Most relevant terms of Optics and Electronics cluster

2000-2003	Score	2004-2007	Score	2008-2010 (Joined SNBUP)	Score	2011-2013 (Joined SNBUP)	Score
external voltage	7.00	nanoscale morphology	16.58	electric vehicle	11.16	semiconductor photocatalysis	13.09
lasing action	5.59	charge collection	15.00	Pulverization	9.64	mose2	12.83
individual single walled carbon nanotube	5.32	improved performance	11.29	graphite anode	9.30	mah g1	9.79
quantum rod	4.55	polymer solar cell	10.49	battery electrode	9.16	visible light photocatalytic hydrogen	8.98
logic function	4.29	bulk heterojunction solar cell	10.04	rechargeable lithium battery	8.53	advanced electrode material	8.89
kilowatts per square centrimetre	3.60	donor acceptor interface	9.61	charge capacity	8.13	robust adhesion	8.42
electrical transport	3.55	charge generation	9.54	energy storage device	7.48	asymmetric supercapacitor	8.35
measurement transport study	3.39	biological labeling	9.12	cycle life	7.41	flexible energy storage device	8.21
low temperature growth	3.31	plastic solar cell	8.30	fascinating property	7,39	superior cyclability	8.21
modules for experiments in stellar astrophysics	3.06	graphene nanoribbon	8.05	supercapacitor electrode material	7.09	high energy lithium ion battery	8.11
density of states	3.02	poly3 hexylthiophene butyric acid methyl ester	7.95	high charge storage capacity	6.81	capacitive energy storage	7.88
laser emission	3.02	semiconducting polymer	7.94	electrochemical energy storage	6.80	new electrode material	7.87
cdse quantum dot	2.80	solid state lighting	7.69	hydrocarbon fuel	6.77	excellent mechanical strength	7.70
dimensional plasmon	2.77	overall conversion efficiency	7.10	capacity fading	6.75	high performance libs	7.66
miniband transport	2.77	multiple exciton generation	7.06	gradual reduction	6.64	nanostructured electrode material	7.27

**Table 4.** Most relevant terms of Synthesis of nanomaterials and bottom-up processes

2000-2003 (Joined Biotechnology & y Biomedicine)	Score	2004-2007	Score	2008-2010 (Joined Optics & Electronics)	Score	2011-2013 (Joined Optics & Electronics)	Score
zno nanowire	20.81	nm wall thickness	11.13	electric vehicle	11.16	semiconductor photocatalysis	13.09
acid methyl ester sensitization	16.34	cd2 ion	9.85	pulverization	9.64	mose2	12.83
	16.28	tio2 nanotube array	9.22	graphite anode	9.30	mah g1	9.79
solar energy conversion	14.13	gold nanocage	8.76	battery electrode	9.16	visible light photocatalytic hydrogen	8.98
catalytic growth	13.28	nm pore diameter	8.76	rechargeable lithium battery	8.53	advanced electrode material	8.89
butyric acid methyl ester shell thickness	12.95	silver nanocube	8.47	charge capacity	8.13	robust adhesion	8.42
	12.77	polyaniline nanofiber	8.31	energy storage device	7.48	asymmetric supercapacitor	8.35
core shell particle	9.93	potentiostatic anodization	8.21	cycle life	7.41	flexible energy storage device	8.21
zno nanorod	9.83	photoanode	7.42	fascinating property	7.39	superior cyclability	8.21
electrospinning	9.55	liberation	7.15	supercapacitor electrode material	7.09	high energy lithium ion battery	8.11
nanobelt	8.93	titania nanotube array	6.80	high charge storage capacity	6.81	capacitive energy storage	7.88
silver nanowire	8.81	block truncation coding	6.79	electrochemical energy storage	6.80	new electrode material	7.87
novel nanostructure	8.81	chemical activity	6.46	hydrocarbon fuel	6.77	excellent mechanical strength	7.70
soil	8.59	lithium ion secondary battery	6.23	capacity fading	6.75	high performance libs	7.66
polyfluorene	8.42	same chemical composition	6.16	gradual reduction	6.64	nanostructured electrode material	7.27

### *Biotechnology and Biomedicine (purple and orange clusters)*

The cluster *Biotechnology and Biomedicine* is linked to *Synthesis of nanomaterials and bottom-up processes* due to its use of this type of materials. It is also quite connected to *Optics and electronics* because of optical measurements, and to *Microelectronics engineering and top-down processes* because such devices are used as systems of detection.

In the [first period](#) of study, this cluster is joined to *Synthesis of nanomaterials and bottom-up processes*, but in the period [2004-2007](#) the two clusters divide



into separate research lines. Then, in the [following period](#), given the scientific advances in Optics and Electronics and the synthesis of nanomaterials and bottom up processes, this cluster splits in two: *Biosensing* (purple cluster) and *Therapeutic biomedicine* (orange cluster). In more recent years ([2011-2013](#)), *Biosensing* has captured more research, possibly because it provides more direct benefits for society.

**Table 5.** Most relevant terms of Biotechnology and Biomedicine

2000-2003 (Joined SNBUP)	Score	2004-2007	Score	2008-2010 (Biosensing)	Score	2008-2010 (Therapeutic biomedicine)	Score	2011-2013 (Biosensing)	Score	2011-2013 (Therapeutic biomedicine)	Score
zno nanowire	20.81	photothermal therapy	9.97	novel glucose biosensor	6.66	abdominal cavity	8.63	chemical class	10.07	marine organism	6.91
acid methyl ester	16.34	unique optical property	8.85	biotechnology application	6.32	significant obstacle	7.28	complex biological environment	5.82	biological identity	6.00
sensitization	16.28	mesoporous silica nanoparticle	8.81	droplet microfluidic	5.47	Harm	7.11	luminescence	5.31	cellular machinery	5.48
solar energy conversion	14.13	protein engineering	8.18	excellent platform	5.25	implantable medical device	6.23	care diagnostic device	5.20	tissue penetration depth	5.41
catalytic growth	13.28	nm nanoparticle	7.97	graphene oxide surface	4.72	Surrogate	6.02	existing camera unit	5.13	unique size	5.22
butyric acid methyl ester	12.95	electrospun nanofiber	7.10	norepinephrine	4.66	vivo delivery	5.32	dioxetane	5.04	ce6	5.08
shell thickness	12.77	cellular toxicity	6.93	complementary dna strand	4.55	Asbestos	5.25	phosphorylation	5.04	photodynamic therapy efficacy	4.72
core shell particle	9.93	arsenite	6.63	tnt detection	4.10	apparent cytotoxicity	5.18	powerful technology	4.26	diseased cell	4.69
zno nanorod	9.83	s aureus	6.45	bioelectronic	4.04	novel form	5.15	microfluidic paper	4.25	modern medicine	4.65
electrospinning	9.55	gram negative bacterium	6.42	background fluorescence	4.03	endosomal compartment	5.12	resource limited setting	4.15	icp ms analysis	4.48
nanobelt	8.93	cancer treatment	6.36	nonenzymatic	4.01	early onset	4.81	aggregation	4.07	high photot	4.25

		ent		glucose sensor				induced emission characteristics		hermal conversion efficiency new era	
silver nanowire	8.81	cancer diagnosis	6.23	wide linear response	3.89	nanoparticle type	4.76	microfluidic paper based analysis devices	4.06		4.17
novel nanostructure	8.81	related technology	6.10	epinephrine	3.82	protein corona	4.66	fluorogen	4.03	controlled drug delivery	4.15
soil	8.59	antibacterial property	6.04	novel graphene	3.78	human exposure	4.48	catecholamine	3.96	vivo biocompatibility	4.08
polyfluorene	8.42	cancer diagnostic	5.85	good electrocatalytic activity	3.75	human cancer cell	4.41	efficient platform	3.89	gelma	4.07

In the final period of study ([2011-2013](#)) the left part of the cluster *Microelectronics engineering and top-down processes* approaches *Biosensing*, as the terms represented here frequently refer to microfluids, commonly used for biodetection. At the same time this cluster becomes less compact, opening toward the right until it is situated parallel to the cluster *Synthesis of nanomaterials and bottom-up processes*, thereby demonstrating its influence in the rest of the disciplines within NST.

#### *Physical and mechanical characteristics of materials (blue and pink clusters)*

The cluster *Physical and mechanical characteristics of materials* could be considered the first research line to be developed in the field of NST. The studies along this line are related with the principals of physics and the study of the mechanical properties or physical characterizations of certain materials in conjunction with NST discoveries. Once these materials were more familiar at the nanometric scale, the line of research slowed down, while other lines began to evolve thanks to the discoveries recently made. Hence, the lines are seen to intersect or interact to some degree. The tendency over the years is for the cluster *Physical and mechanical characteristics of materials* to move

away from the rest, although it still shares limited activity with *Optics and Electronics*, *Synthesis of nanomaterials and bottom-up processes* and *Microelectronics engineering and top-down processes*. The interaction can be traced to the employment of materials common to all the clusters, yet the part dedicated to the study of mechanical properties of materials tends toward isolation.

**Table 6.** Most relevant terms of Microelectronics engineering and top-down processes

2000-2003	Score	2004-2007	Score	2008-2010	Score	2011-2013	Score
organic thin film transistor	11.50	hydrophilic polymer	7.36	few layer graphene films	16.71	rich physic	16.04
nonvolatile memory	8.60	novel nanoscale	7.17	transparent conducting film	15.10	wse2	12.19
optical application	7.43	Superhydrophilicity	5.95	exciting potential	13.48	ptb7	11.65
design consideration	5.52	new architecture	5.66	scalable technique	13.45	mos2 monolayer	11.02
ferroelectricity	5.36	microscale device	5.36	graphene electrode	12.58	bilayer mos2	10.10
optical switch	4.95	superhydrophobic coating	5.12	nitrogen doped graphene	12.14	entire visible spectrum	9.65
luminescence efficiency	4.20	high gain	4.94	arbitrary substrates	11.20	standard am	9.47
molecular monolayer	3.78	Superhydrophobicity	4.75	large scale growth	10.99	mos2 transistor	9.08
alkyl	3.71	further optimization	4.57	liquid phase exfoliation	10.80	ionic motion	8.71
energy consumption	3.61	optical coherence tomography	4.19	individual graphene sheet	10.62	terminology	8.57
carbon nanotube	3.44	continuous flow separation	4.14	large area graphene	10.18	efficiency limitation	8.31
field effect transistor	3.36	enhanced mixing	4.06	opto electronic property	10.02	valley polarization	8.14
strontium titanate	3.34	Crust	4.03	thick sheet	9.17	efficient polymer solar cell	8.03
atomic force microscopy	3.19	bath temperature	3.99	graphene oxide film	9.04	reduced charge recombination	7.92
cantilever	2.97	lithographic approach	3.85	single sheet	8.93	pec water splitting	7.80
conductive substrate							
charge fluctuation							

During the period [2000-2003](#) this cluster lies at a great distance from the other research lines. Another singular aspect of this cluster is its division into two lines. Namely, *Physical characteristics of materials* (pink cluster, top left), and *Mechanical characteristics of materials* (blue cluster, lower left). We also see a distance from the other research lines identified. Yet in the following period ([2004-2007](#)) the two lines fuse into a single cluster, and remain attached until the end of the period.

**Table 7.** Most relevant terms of Physical and mechanical characteristics of materials cluster

2000-2003 (Mechanical)	Score	2000-2003 (Physical)	Score	2004-2007	Score	2008-2010	Score	2011-2013	Score
solid oxide fuel cell	5.11	magnesium alloy az31	5.66	mechanical reinforcement	5.95	enhanced strength	6.99	local property	5.76
stage process	3.66	continuous dynamic recrystallization	3.96	simultaneous increase	5.07	effective reinforcement	3.74	video recording	5.20
high capacity	3.54	ultrafine grained	3.94	annealing time t	3.24	watt per meter kelvin	2.92	strong size dependence	3.73
spark plasma	3.52	accumulative roll bonding	3.08	filler material	2.98	dimensional finite element simulation	2.84	tafel analysis	3.09
high temperature stability	3.24	peak value	2.96	nanotube polymer composite	2.84	concrete	2.54	random texture	2.57
hall petch relationship	3.21	nanocrystalline metal	2.69	recrystallization mechanism	2.59	ultimate strength	2.50	si particle	2.45
yttrium oxide	3.17	recrystallization mechanism	2.46	ultrafine grain size	2.54	macromolecular structure	2.47	relevant temperature range	2.31
columnar grain structure	3.03	flow instability	2.45	low ductility	2.41	disclination	2.18	optimum balance	2.25
coating property	3.02	continuous recrystallization	2.43	good electrical conductivity	2.40	large strain	2.09	primary focus	2.20
friction stir weld	2.97	route c	2.43	ultrafine grained microstructure	2.38	damaged region	2.09	outstanding mechanical property	2.16
solid matrix	2.97	high pressure torsion	2.39	inducing	2.31	minimally	2.07	segregation behavior	2.16
multicomponent system	2.92	equal channel angular pressing	2.34	surface mechanical attrition treatment	2.29	major mechanism	2.04	thick sheet	2.10
fold symmetry	2.90	silicon	2.31	microwave sintering	2.25	extrusion texture	2.02	multistep	2.08
load transfer	2.86	nanotube hot deformation behavior	2.30	deformability	2.20	crystal form	1.86	Lmc	1.99
automotive industry	2.85	grain size dependence	2.19	rapid heating	2.08	higher yield strength	1.86	cyclic strain	1.96

### *Organic electronics (light blue cluster)*

This cluster only appears in the period [2008-2010](#), owing to the use of organic materials within the realm of NST research. This causes it to occupy a position nearby the cluster *Synthesis of materials and bottom-up processes*.

However, the line of research eventually disappears, absorbed into the cluster *Microelectronic engineering and top-down processes* during [2011-2013](#).

**Table 8.** Most relevant terms of Organic electronics cluster

2008-2010	Score
Minority carrier diffusion length	11.72
Polymer donor	8.27
Vertical phase separation	8.19
High absorption coefficient	7.87
Fullerene acceptor	7.61
Polymer morphology	6.14
Solvent free ionic liquid electrolyte	5.98
Reduced graphene oxide film	5.97
Photoconversion efficiency	5.76
Solution processed	5.75
Electron pathway	5.72
Functionalized graphene	5.52
Bulk heterojunction solar cell	5.49
Particulate film	5.46
Diketopyrrolopyrrole	5.46

#### 4. Conclusions

By means of CitnetExplorer, we have analyzed the intellectual structure of Nanoscience & Nanotechnology, identifying the seminal papers and key documents of all NST journals contained in the JCR Science Edition during the period 2000-2013.

In view of the influence that the most-cited works have exerted over the years studied, we conclude that seven groups can be discerned within the intellectual structure of NST. The articles making up these groupings are

essential papers of reference for the development of the discipline, and they are recognized as such through citations by the community of scientists. The underlying structure visualized here shows that even a limited and recent time period serves to elaborate the genealogy of a field such as NST, as the scientific culture always leaves footprints behind—that is, new authors look to their predecessors for foundational knowledge (Bayer et al. 1990). Citation habits are strongly conditioned by the magnitude of scientific progress, as reflected by the articles by Iijima about carbon nanotubes, or the experiments of Novoselov and colleagues with graphene. Such crucial steps in the development of NST give rise to new subject areas that are eventually consolidated through an array of articles, either within or surrounding the intellectual sphere of *carbon nanomaterials*.

Deserving mention as an outstanding example is the appearance of a thematic area related with *organic electronics*, in this case attracting little attention among the scientific community, with only one article in the map cluster.

In our opinion, the structures identified and displayed in this work make manifest certain consolidated subject areas, stemming from works that report authentic scientific breakthroughs, or key methodological proposals. There is evident consensus regarding the significance and usefulness of such contributions to NST.

Many of the documents identified in this study differ from those described by Kostoff and colleagues (2006, 2007a), who took into account the citation of the documents of all scientific fields. Our work resorted to citation of the documents in the category NST of the WoS, meaning that we only accounted for citation by experts in the discipline. Visualization techniques and *co-word* analysis, in this case from titles and abstracts, allowed us to identify and project the evolution of the main research lines developed in NST from 2000 up to 2013.

The research lines traced are evidence of output exploring the behavior and phenomena at the nanoscale, together with the creation of new materials and their diverse applications. The profile of NST, accordingly, can be summed up as a young discipline in steady expansion, still needing some time to secure its foundations. This would explain why research lines such as *Optics and electronics*, *Synthesis of nanomaterials and bottom-up processes* or *Physical and mechanical characteristics of materials* maintain a constant flow of output. In contrast, *Biotechnology and Biomedicine* and *Microelectronics engineering and top-down processes* undergo a bit of a boom, perhaps because there are greater health-related social benefits associated with these topics. It could also be that these lines will produce important economic benefits in the near future. New research lines arise with the applications of nanomaterials together with the trend of working with organic materials, as seen in the case of *Organic electronics*. However, no research line related with NST toxicology in biological or environmental contexts was detected. Many words related to this field —nanoparticle toxicity, nanotoxicity, ecotoxicity and so on— are included in the clusters *Biotechnology and Biomedicine: Biosensing and Therapeutic biomedicine*. This line will no doubt emerge and gain strength in the coming years, with new developments to generate methods for the safe production, use and elimination of nanomaterials (Nel et al. 2006).

When the number of documents published in a given research area is lower than in others, the number of citation is understandably low as well. Here we could evoke the case of Nanotoxicity. While some National Science Foundation (NSF) funded centers investigate the toxicity of nanomaterials (e.g. the Center for the Environmental Implication of Nanotechnology, Center for Sustainable Nanotechnology), overall the production of scientific literature in this area that does not strictly correspond to *Biotechnology and Nanomedicine* or *Synthesis of nanomaterials and bottom-up processes* may be low because its scope of action is limited. It may also be that scientific production in this specific realm is not registered in the leading multidisciplinary database of WoS. We might therefore affirm that our work

has not yet come to an end along this research line: one of the journals that our search strategy includes is *Nanotoxicology*, a specialized journal in this field. On the other hand, one journal is not enough to provide insightful clues into a field of knowledge. On a broader panorama, as the science maps show, all the terms associated with Nanotoxicity appear inside the clusters *Biotechnology and Nanomedicine* or *Synthesis of nanomaterials and bottom-up processes*, not as a separate research line.

The lack of scientific literature in the wake of certain research lines and the low citation rate harvested by them could explain why most seminal papers identified in this manuscript pertain to the field of technology development.

Both the intellectual and the cognitive structures identified illustrate how NST continues to occupy a largely interdisciplinary scientific area. Indeed, its development depends on the knowledge that comes from physics, chemistry and materials science, as displayed by the science maps. This is no novelty, having been endorsed by previous analyses (Meyer and Persson, 1998; Schummer, 2004; Porter and Youtie 2009; Jo et al. 2016), which to some extent demonstrate the convergence and validity of the scientometric methodology used in this study. In short, however, the present endeavor strives to trace the research lines of NST and thereby show how research in the area has changed over time. It is our hope that this study will become a useful tool of reference for the NST scientific community, revealing at a glance essential research lines in the light of landmark papers. Additionally, the methodology used in this study can be implemented in any other scientific field so as to explore its intellectual and cognitive structure.

## **5. Limitations and future efforts**

We must acknowledge specific problems inherent to map elaboration. Firstly, when working with a free and non-controlled language for the titles and abstracts of the documents studied, there are inevitable problems of synonymy, acronymy, and plural vs. singular denoting a single concept.



Secondly, the non-use of controlled language may have led to an absence of keywords that could define a research line quite well, but were not included in the titles or abstracts that we worked with. A potential solution for the future is to use keyword authors and index keywords to create science maps. This would necessarily entail using both controlled and non-controlled language, because the use of controlled language alone implies an absence of terms presently used in NST (Braam et al. 1991b).

Another limitation is related to the specific knowledge of the studied subject (NST) that will be covered in future works. No doubt consultation with experts in the scientific field would solve this limitation, since the opinion, review and comments from them would allow us to guarantee the results, as well as reinforce, reorganize, reclassify, and deepen the thematic specialization, and therefore delimit in a clearer and more concise way the groups pertaining to the network and co-word maps.

Looking once again toward the future, we believe that the design of search strategies will be improved, embracing journals that cover all the research lines that NST touches upon, and not merely the journal set ascribed under WoS. Furthermore, the methodology put forth here may be exported to study the category NST in other databases of a multidisciplinary character, where this category has been previously identified. It could also be extrapolated to other thematic fields. In addition, overlay techniques may be used in conjunction with the method. To a certain extent, the future of bibliometric techniques for scientific categorization and exploration may be foreseen through similar efforts.

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## **Appendix A. Abbreviated journal titles (JCR) query**

SO=(ACM J EMERG TECH COM OR ACS APPL MATER INTER OR ACS NANO OR ADV FUNCT MATER OR ADV MATER OR AIP ADV OR BEILSTEIN J NANOTECH OR BIOMED MICRODEVICES OR BIOMICROFLUIDICS OR BIOSENS BIOELECTRON OR CURR NANOSCI OR DIG J NANOMATER BIOS OR FULLER NANOTUB CAR N OR IEEE T NANOBIOSCI OR IEEE T NANOTECHNOL OR IET NANOBIOTECHNOL OR INT J NANOMED OR INT J NANOTECHNOL OR J BIOMED NANOTECHNOL OR J COMPUT THEOR NANOS OR J EXP NANOSCI OR J LASER MICRO NANOEN OR J MICRO-NANOLITH MEM OR J MICROMECH MICROENG OR J NANO RES-SW OR J NANOBIOTECHNOL OR J NANO ELECTRON OPTOE OR J NANOMATER OR J NANOPART RES OR J NANOPHOTONICS OR J NANOSCI NANOTECHNO OR J PHYS CHEM C OR J PHYS CHEM LETT OR J VAC SCI TECHNOL B OR LAB CHIP OR MAT SCI ENG A-STRUCT OR MATER EXPRESS OR MICRO NANO LETT OR MICROELECTRON ENG OR MICROELECTRON J OR MICROELECTRON RELIAB OR MICROFLUID NANOFLUID OR MICROMACHINES-BASEL OR MICROPOR MESOPOR MAT OR MICROSYST TECHNOL OR NANO OR NANO ENERGY OR NANO LETT OR NANO RES OR NANO TODAY OR NANO-MICRO LETT OR NANOMATER NANOTECHNO OR NANOMED-NANOTECHNOL OR NANOMEDICINE-UK OR NANOSC MICROSC THERM OR NANOSCALE OR NANOSCALE RES LETT OR NANOSCI NANOTECH LET OR NANOTECHNOLOGY OR NANOTOXICOLOGY OR NAT NANOTECHNOL OR PART PART SYST CHAR OR PHOTONIC NANOSTRUCT OR PHYSICA E OR PLASMONICS OR PRECIS ENG OR RECENT PAT NANOTECH OR REV ADV MATER SCI OR SCI ADV MATER OR SCRIPTA MATER OR SMALL OR SYNTH REACT INORG M OR WIRES NANOMED NANOBI)

## Appendix B. Nodes and citations

<b><i>Node</i></b>	<b><i>Year</i></b>	<b><i>Source</i></b>	<b><i>Citation</i></b>
Iijima	1991	Nature	3183
Perdew	1996	Physical Review Letters	3072
Novoselov	2004	Science	2856
Geim	2007	Nature Materials	2169
Kresse	1996	Physical Review B	1997
Oregan	1991	Nature	1779
Xia	2003	Advanced Materials	1531
Kresse	1999	Physical Review B	1529
Frisch	2004	Gaussian 03 Revision	1492
Kresse	1996	Computational Materials Science	1462
Huang	2001	Science	1444
Monkhorst	1976	Physical Review B	1441
BlochI	1994	Physical Review B	1438
Kresge	1992	Nature	1343
Alivisatos	1996	Science	1311
Daniel	2004	Chemical Reviews	1258
Novoselov	2005	Nature	1201
Baughman	2002	Science	1197
Lee	1988	Physical Review B	1196
Becke	1993	Journal of Chemical Physics	1172
Hummers	1958	Journal of the American Chemical Society	1135
Murray	1993	Journal of the American Chemical Society	1077
Johnson	1972	Physical Review B	1075
Cui	2001	Science	1063
Pan	2001	Science	1041
Wagner	1964	Applied Physics Letters	1029
Nie	1997	Science	1029
Kresse	1993	Physical Review B	1026
Zhang	2005	Nature	1026
Sze	1981	Phys Semiconductor Devices	1010
Chan	1998	Science	1001
Bruchez	1998	Science	996
Kelly	2003	Journal of Physical Chemistry B	992
Zhao	1998	Science	951
Law	2005	Nature Materials	950
Stankovich	2006	Nature	918
Fujishima	1972	Nature	913
Kim	2009	Nature	903
Gratzel	2001	Nature	890

Li	2009	Science	889
Michalet	2005	Science	876
Ferrari	2006	Physical Review Letters	875
Kong	2000	Science	870
Perdew	1992	Physical Review B	861
Hoffmann	1995	Chemical Reviews	845
Vanderbilt	1990	Physical Review B	844
Burda	2005	Chemical Reviews	841
Beck	1992	Journal of the American Chemical Society	827
Lee	2008	Science	825
Perdew	1992	Physical Review B	818
Decher	1997	Science	799
Tans	1998	Nature	786
Castro Neto	2009	Reviews of Modern Physics	786
Morales	1998	Science	780
Huynh	2002	Science	777
Saito	1998	Phys Properties Carb	759
Geim	2009	Science	750
Kohn	1965	Physical Review	736
Wang	2006	Science	724
Li	2008	Nature Nanotechnology	724
Stankovich	2007	Carbon	719
Kreibig	1995	Optical Properties M	713
Frisch	2009	Gaussian 09 Revision	708
Love	2005	Chemical Reviews	702
Asahi	2001	Science	700
Barnes	2003	Nature	697
Peng	2000	Nature	690
Soler	2002	Journal of Physics: Condensed Matter	681
Medintz	2005	Nature materials	672
Novoselov	2005	PNAS	659
Schedin	2007	Nature Materials	634
Yu	2003	Chemistry of Materials	633
Bard	2001	Electrochemical Meth	632
Berger	2006	Science	629
Kresse	1994	Physical Review B	628
Troullier	1991	Physical Review B	621
Bohren	1983	Absorption Scattering	619
Li	2008	Science	616
Li	2005	Nature Materials	614
Kneipp	1997	Physical Review Letters	607

## **Capítulo 10. Coping with the delineation of emerging fields: Nanoscience and Nanotechnology as a case study**

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### **Abstract**

Proper field delineation plays an important role in scientometric studies, although it is a tough task. Based on an emerging and interdisciplinary field — nanoscience and nanotechnology— this paper highlights the problem of field delineation. First we review the related literature. Then, three different approaches to delineate a field of knowledge were applied at three different levels of aggregation: subject category, publication level, and journal level. Expert opinion interviews served to assess the data, and precision and recall of each approach were calculated for comparison. Our findings confirm that field delineation is a complicated issue at both the quantitative and the qualitative level, even when experts validate results.

### **1. Introduction**

Field delineation<sup>1</sup>, which consists of assigning journals or publications to fields, tends to be the first stage undertaken in bibliometric or scientometric studies of fields (Zhao, 2009). Proper field delineation is important for researchers who study the structure and dynamics of a field, and it is fundamental for information retrieval in the research areas of bibliometrics and scientometrics. It is also needed when designing reliable and solid tools for rankings and domain analysis, highly valuable in science policy design and science evaluation processes (Gómez-Núñez et. al. 2014). Indeed, the relevance of such studies will depend on the quality of their delineation. Specific challenges lie in the process of delineating emerging and/or interdisciplinary fields, for example, in the retrieval of relevant data with high

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<sup>1</sup> The terms field delineation, subject classification, subject category delineation, subject delineation, thematic delineation, and discipline delineation are used interchangeably throughout this text.

precision and hefty recall, and the construction of a core journal or publication set to comprise a field (Milanez et al., 2016).

Likewise, delineating scientific fields before developing disciplinary subject classification schemes may involve empirical and pragmatic techniques, or other automated procedures based on statistics and computerized methods. However, the hierarchy of sciences, where consensus within scientific community of a field can be easily reached at the core level (where theories or methods are fully accepted), but not at the research frontier level (where the research is conducted) (Cole, 1983), provides a framework to understand the diversity of a discipline since it reflects the level of scholarly consensus and shows natural-social dichotomies (Fanelli & Glänzel, 2013). This consensus can involve not only cognitive aspects or complexity of a subject matter, but also sociological aspects. Therefore, the definition of a field derives from its scientific content as well as from the association and interaction (social, professional or by publishing) of its researchers. A lack of cohesion in a field can be considered as a factor to detect an emerging field (Casadevall & Fang, 2015).

Several methods may be used to delineate fields. Subject-classification schemes, made up mainly of scientific journals, are one information retrieval strategy that can help to collect a relevant document set for field delineation. This is the classification system used by the top two multidisciplinary bibliographical databases, Scopus and Web of Science (WoS). They assign scientific journals to categories taking into account journal title and scope, as well as journal citation analysis. Although subject-classification schemes may define a broad field, this type of delineation encounters limitations regarding the level of detail, multidisciplinary journals, and interdisciplinary research published in a variety of journals, defying disciplinary boundaries (Zhao, 2009); in such cases, the retrieved document set contains considerable noise affecting both precision and recall (Glänzel, 2015). In order to offset these



limitations, an alternative method may be used to delineate by assigning not only journals but also publications to categories (Glänzel & Schubert, 2003).

The most common information retrieval archetype used for field delineation entails the translation of an information need into a query or a set of queries. The application of complex search strategies based on lexical terms (keywords and phrases) is most widely used to collect a document set related to a field/domain, especially in emerging and interdisciplinary fields, because it can effectively cover most aspects of the field (Glänzel, 2015). This method has been progressively fine-tuned, and can now be considered a hybrid lexical-citation method. At the seminal level, it may be used to appraise a field of literature, or core journal publications, through retrieval by lexical queries. The initial seed set is then extended by citation analysis among publications using different parameters. However, this process becomes problematic when, for instance, the use of common terms bears a negative influence on precision yet a positive one on recall. Total recall can also be affected because the borders of fields are sometimes difficult to define; and the help of experts in the field to design lexical queries can produce a specialization bias, leading to a skewed and superficial overview of the field/domain (Zitt, 2015).

Extensive research has shown that clustering analysis is a valuable and popular method applicable at journal and publication level, in a wide variety of scientific fields (Zitt & Bassecouard, 2006; Bassecouard et al., 2007; Gómez-Núñez et al., 2014). Boyack and Klavans (2010, 2013) use hybrid methods that combine different types of citation relations and conclude that the approach generates accurate clusters.

More recent attention has focused on the use of multidisciplinary classification systems at the publication level, as established by Waltman & van Eck (2012). It is based on direct citation relations between publications from WoS and clusters them into research areas organized in a three-level hierarchical structure. Delineating at the publication level more accurately matches the

current structure of scientific research in a field. Accordingly, the classification system of publications could help define a journal level system, but it might prove problematic the other way around. Field delineation at the level of publication is one possible solution when facing the limitations involved in classification at the level of journal.

In the same line, Klavans and Boyack (2017) introduce a detailed classification system at the topic level with around 100,000 topics that have been applied in Scopus. The Scopus documents set is divided into topics by the clustering of direct citation links. Then, a measure to rank the topic prominence in science is applied to identify those topics that reveal supply and demand in the science systems. Field delineation at this topic level offers the advantage of predicting if a topic will grow or decline, and its contribution to the dynamics of the science, in terms of the funding received.

Recent research has compared different journal and publication classification systems (Shu et al., 2019). These authors claim the necessity of developing robust and accurate publication and journal classification systems. An increase in the number subjects included in a publication journal classification system has an effect in the accuracy and can reduce the misclassification of papers. The same effect is produced in a journal classification system when it includes broad or high-level disciplines instead of many disciplines.

Nowadays, Nanoscience and Nanotechnology is an area holding vast technological and social potential for the community, presenting advancements for industry, health, the environment, and security. It therefore attracts great policy interest. Thus, NST has been included as a strategic area with an innovative and economic potential in many research and development plans, even worldwide, like the EU Research and Innovation Programme known as Horizon 2020<sup>2</sup>, the National Science Foundation<sup>3</sup> and the National

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<sup>2</sup> [ec.europa.eu/programmes/horizon2020/en/what-horizon-2020](https://ec.europa.eu/programmes/horizon2020/en/what-horizon-2020)

<sup>3</sup> [www.nsf.gov](https://www.nsf.gov)

Nanotechnology Initiative <sup>4</sup>. Previous efforts have delineated NST from different perspectives (Zitt & Bassecouard, 2006; Leydesdorff & Zhou, 2007; Mogoutov & Kahane, 2007; Grieneisen & Zhang, 2011; Arora et al. 2013, 2014), but to date no comparison of these methods has been performed. The current study compares three different approaches to delineate the emerging field of NST, shedding new light on the key problems that underlie emerging field delineation.

### *1.1. Delineation of Nanoscience and Nanotechnology*

Nanoscience and Nanotechnology (henceforth NST) constitutes an interdisciplinary and emerging domain that embraces physics, chemistry, materials science, engineering, and more. Since the 1990s, many works have attempted to delineate NST by using different perspectives, e.g. thematic delineation or bibliometric techniques.

Various lexical queries have been proposed for gathering the data set to study NST, including:

- 1) The prefix *nano*, to harvest all publications that include it within their title (Meyer et al., 2001; Tolles, 2001; Dunn & Whatmore, 2002);
- 2) A combination of *nano* prefix and representative keywords of NST, excluding those terms that include the *nano* prefix but have nothing to do with NST (Glänzel et al., 2003; Noyons et al., 2003; Mogoutov & Kahane, 2007; Porter et al., 2008).

The drawback of searching based on the *nano\** prefix alone is that publications without a prefix are not retrieved (for instance, biotechnology publications). In addition, some NST keywords such as fullerenes or graphene are excluded. The second search strategy is supported by experts' opinion to include or exclude keywords, yet it tends toward bias, because the experts

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<sup>4</sup> [www.nano.gov](http://www.nano.gov)

may include keywords associated with their particular field of knowledge (Huang, Notten, & Rasters, 2011).

An early work proposing a lexical query to study NST is that by Braun, Schubert & Zsindely (1997). These authors harvested articles with the prefix *nano* from 1986 to 1995 in order to analyze the growth of nanotechnology. Some years later, Kostoff and colleagues (2006) studied NST to identify its thematic structure. They recreated the genealogy of NST in terms of the most important works behind the development of NST based on the assumption that they would be highly cited. Zitt & Bassecouard (2006) delineate NST literature by combining lexical queries and citation analysis, additionally using a set of parameters to highlight relevance and reduce noise. A worldwide view of the technical structure and infrastructure of scientific production in NST drawn up by Kostoff, Koytcheff and Lau (2007) introduced us to the most productive and highly impacting countries.

One important finding two decades ago is that journals focusing on physics published the greatest number of NST publications, followed by interdisciplinary journals (Meyer & Persson, 1998). The search involved articles with the prefix *nano* in their titles between 1991 and 1996 retrieved from the Science Citation Index, distributing them according to the journal classification scheme proposed by Hicks & Katz (1996).

Schummer (2004) ran a co-author analysis of over 600 articles published in *nano* journals in 2002 and 2003. The results showed that most NST journals include publications by authors with just one disciplinary affiliation, especially by physicists. He furthermore explored the speed at which the scientists and engineers from different disciplines, institutions and countries take part in NST research, and whether the development of NST involves new means or levels of multi and interdisciplinary research, or institutional and geographical collaboration patterns. Results indicated that there are no particular patterns

or stable levels of multi- or interdisciplinary research —while interaction exists, it shares little more than the prefix *nano*.

Bassecoulard, Lelu and Zitt (2007) looked into NST as a multidisciplinary field of knowledge by means of a classification of publications in thematic clusters connected by the similarity of their references. With an NST data set from 1999 to 2003, they evidenced a moderate level of multidisciplinary, though just a few publications in physics and chemistry were at the root of that multidisciplinary.

The NST journals with the *nano* prefix in their titles included in the Journal Citation Report (JCR) from 25 countries were studied by Andrievski and Klyuchavera (2011). New journals in NST were found to come from fields such as nanobiology, nanomedicine, nanobiomedicine, and nanobiotechnology, whereas the bulk of scientific production in NST was published in classic natural-science and engineering journals.

Huang and his collaborators (2011) conducted a review of the nanotechnology literature that had analyzed publications and patents. They identified pros and cons of the different search strategies carried out for nanotechnology delineation: keyword queries and all their improvements, citation analyses, and the use of a core journal set to identify articles. As most of the search strategies for nanotechnology delineation shared a core keyword set, the results obtained in terms of main areas and journals in nanotechnology proved similar. Their lexical queries were designed in view of the search strategy suggested by Glänzel et al. (2003). The other search strategy was based on the use of the top 10 journals in nanotechnology; however, it did not provide a solid delineation because many nanotechnology papers are published in multidisciplinary journals.

A number of attempts to improve keyword queries for the retrieval of NST publications (Kostoff et al., 2006; Kostoff, Koytcheff, & Lau, 2006; Mogoutov & Kahane, 2007; Zucker et al., 2007; Maghrebi et al., 2011) rely on a data set

harvested using an initial keyword search strategy and a selection of keywords based on the relevance of those terms.

On the one hand, Maghrebi et al. (2011) used keyword queries proposed by Warris (2004) to study precision and recall of the keywords by analyzing the articles of 2008 in WoS. On the other hand, the combination of keyword queries and citation analysis used to delineate NST can be seen as a highly effective approach, since it increases precision and recall, reducing the noise of information retrieval (Zitt & Bassecoulard, 2006). Although keyword queries are still used, subjectivity is reduced because expert consultation is not necessarily required (Huang et al., 2011).

Another search strategy described in the literature on NST delineation involves the use of core journals: Leydesdorff & Zhou (2007) identified a set of 10 relevant journals in NST using betweenness centrality as a measure of the interdisciplinarity of scientific journals, with visualization techniques based on citation analysis of journal titles. In addition, they analyzed Nanotechnology patents from the U.S. Patent and Trade Office (USPTO) to determine whether the patents contain references to non-patent literature. Such references were found to be too general to define a set of key journals, and NST appeared to arise from the interrelation between Physics and Chemistry. The drawback of this method, as opposed to retrieval based on keyword queries and citation analyses, is that only a small portion of the NST literature (thematic corpus) is covered.

Detailed examination and update of the nano search strategy by Wang et al. (2019) reported that the dynamism of nanotechnology forces to constantly review its terminology to conduct accurate analyses of the field and detect emerging nano research terms. They suggested a procedure to harvest a proper nano data set that combined nano documents retrieved by lexical queries and nano documents retrieved by NST WoS subject category. The

outcomes evidence that many of the nano research is not covered by the NST WoS subject category.

The present contribution stems from a search strategy combining several approaches previously described for the recovery of NST documents, launched in the Scopus database. Our objective was to derive an NST journal classification in the SCImago Journal and Country Rank (SJR) and in the SCImago Institutions Rankings (SIR) portals based on the Scopus data. All NST articles, conference papers, and reviews contained in Scopus were recovered for the year 2010. Subsequently, a citation analysis of the most cited journals was carried out based on the references of the analyzed documents. The journals that reflected over 1% of total citation were selected (A), excluding multidisciplinary journals. In order to identify the journals that contained the prefix *nano* in the title covered in Scopus, another search was launched in the database, taking only those journals with a *nano* prefix that had received at least one citation in 2010 (B). The sum of journal sets A and B determined the NST core journals (Muñoz-Écija et al., 2013).

## **2. Objectives**

The overall motivation behind this study was to keep working on optimizing and updating the NST journal classification in the framework of the SCImago Journal & CountryRank (SJR) portal. As there is no unique and infallible means of field delineation, the present paper seeks to highlight certain issues involved in delineating emerging fields, using NST as a study case. Our main aim is not to offer a new method or solution, but to explore and compare three approaches so as to show how field delineation varies under the different methods, and aspire to the following specific objectives:

- To update the literature review of field delineation in NST;
- To unify search strategies when harvesting the NST collection;
- To set up a framework for comparing and combining approaches at the journal level through a seven-step procedure;

- To use two distinct value data sources, Scopus and WoS, to delineate an emerging field;
- To include validation by experts in the NST field.

### 3. Material and Method

Two different databases were used to harvest the data set: Scopus and WoS Core Collection (SCI-Expanded, SSCI, and A&HCI indexes). These two databases are widely held to be the most formal data sources in terms of publications because they cover a huge journal collection, and they store publication activities including various reliable indicators (Park et al., 2016). Moreover, two separate classification journal systems were employed to obtain journal lists: Journal Citation Reports (JCR) and SCImago Journal & Country Rank (SJR) in their 2015 and 2016 versions. The time period chosen was 2008-2015 because it marked a certain stability in NST scientific output (Muñoz-Écija et al., 2017).

In analyzing these data sets, three alternative approaches were applied: 1) at category level ( $A_1$ ); 2) at publication level ( $A_2$ ); and 3) at journal level ( $A_3$ ).

#### 3.1. Approach 1: Delineation at category level ( $A_1$ )

To date, WoS is the only multidisciplinary database that includes NST as a subject category. Assignment of journals to subject categories in WoS is the result of a heuristic method based on citation data, long regarded as perhaps “*the best way*” to delineate fields in journal terms (Pudovkin & Garfield, 2002). Under this approach, 88 journals contained in the WoS NST subject category were selected. To do so, this subject category in the JCR Science Edition 2015 and 2016 were chosen (Appendix 1a). Because Scopus does not include the subject category NST among their subject areas, field delineation for NST was drawn in the SCImago Journal and Country Rank portal using subject classification in conjunction with citation- and query-based approaches (Muñoz-Écija et al., 2013). A total of 86 journals contained in SJR



in the years 2015 and 2016 were selected for used in approach  $A_3$ , excluding ceased/discontinued journals (Appendix 1b).

### *3.2. Approach 2: Delineation at publication level using micro-level fields ( $A_2$ )*

This second approach was applied for field delineation in terms of publications as described in Waltman and van Eck (2012). This classification system is used by the Centre for Science and Technology Studies (CWTS) Publication Level Classification System, that comprises more than 4,000 categories, also known as micro-level fields. The search strategy relied on the in-house version of WoS from the CWTS of Leiden University (Appendix 2) to obtain an initial NST data set. The strategy evolves from one used earlier to construct the NST category in SJR and SIR portals (Muñoz-Écija et al., 2013), based on lexical queries combining the *nano* prefix and a list of keywords related to *nano* by means of Boolean operators. All the keywords queries were designed taking into account lexical queries reported elsewhere (Kostoff, Koytcheff, et al., 2006b; Grieneisen & Zhang, 2011; Maghrebi et al., 2011; Arora et al., 2013). For the period covered by the CWTS classification, 2000-2016, the number of articles and reviews retrieved amounted to 1,005,801.

This total of 1,005,801 publications was spread out into micro-level fields that included at least one publication from the NST publication set 2008-2015. These publications were located at 3,433 micro-level fields. The percentage of overlapped publications was calculated by dividing the number of matched publications per micro-level field by the total number of publications in each micro-level field. We believe that the occurrence of publication in relevant micro-fields that come to represent a field can be regarded as a publication overlap having a minimum frequency of 60% in each cluster. Consequently, only micro-level fields with a threshold equal to or greater than 0.6 of overlapped publication were selected. Afterwards, the number of publications per journal covering the 35-selected micro-cluster were calculated (3,851 journals and 332,739 publications in total), as was the total number of publications per journal in the WoS collection for the same time period. The

percentage of publications per journal is thus approximated by dividing the two values. Journals over the 0.2 threshold of publication per journal and over 50 publications were extracted. A list of 78 journals was made, but two turned out to be the same journal that had changed its name. Also, one “ceased” journal was identified using this approach. The final number of journals was therefore 76.

### 3.3. Approach 3: Delineation at journal level ( $A_3$ ) / Lexical query

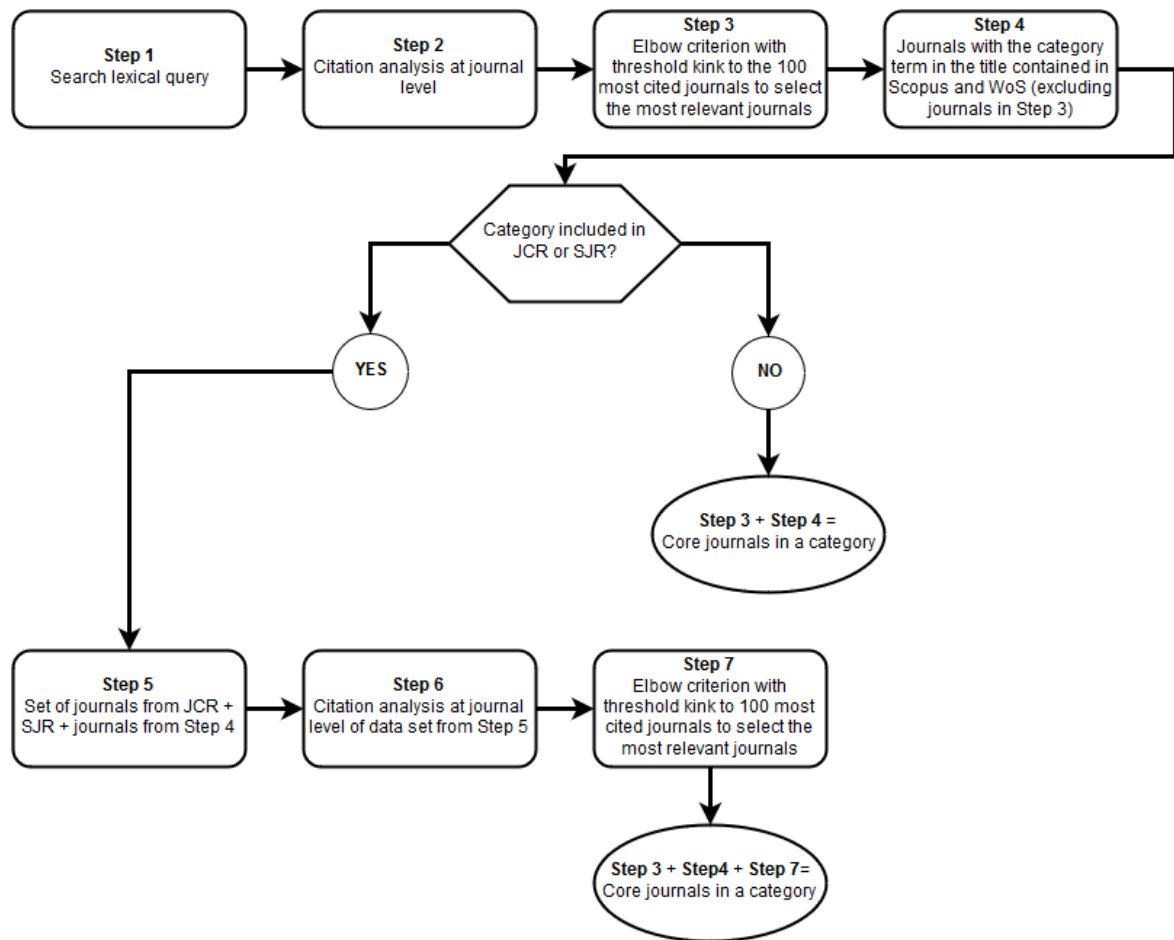
This approach builds on a previous work (Muñoz-Écija et al., 2013), but improves upon the design for an optimal lexical query to harvest the NST data set and implements a statistical method to estimate unknown parameters.

#### Step 1. Searching lexical query

[Figure 1](#) shows a sequence of steps at the journal level. It starts with retrieving the data set from Scopus and WoS databases by applying the NST search strategy (Appendix 2). All document types published from 2008 to 2015 were considered for both databases ([Table 1](#)).

**Table 1.** Data retrieved by Approach 3 ( $A_3$ )

Database	Period	Document type	Number of publications
Scopus	2008-2015	All	902,082
WoS	2008-2015	All	711,464



**Figure 1.** Steps in field delineation at the journal level

### *Step 2. Citation analysis*

We determine the set of cited journals in NST publications retrieved in each database. Before that, the multidisciplinary cited journals included in the Multidisciplinary subject category of JCR were removed, along with those in the General subject category of SJR. This step was based on the assumption that multidisciplinary journals publish articles of many different fields and cannot be considered as journals pertaining to a specific field of knowledge (Narin, 1976). The multidisciplinary of journals might also be studied as an indicator in the *citing* dimension rather than in the *cited* one (Leydesdorff, 2007).

### Step 3. Elbow criterion with threshold kink

After calculating the percentage of citation for each cited journal, the elbow criterion was used to choose the most representative journals. To formalize the visual procedure of an elbow criterion, we employ a statistical procedure that is extensively used in economics and related fields. In particular, we estimate a threshold model with a kink and two straight lines connected at this kink, based on applying the method known as Ordinary Least Squares (OLS) that minimizes the distance of points to a fitted line by minimizing the squared distance to each line. For each subsection, we relate different values of the variable  $x$  (most cited journals) to the variable  $y$  (percentage of citation) and determine parameters  $a$  and  $b$  by the OLS technique, which leads to a straight line (Greene, 2012), where:

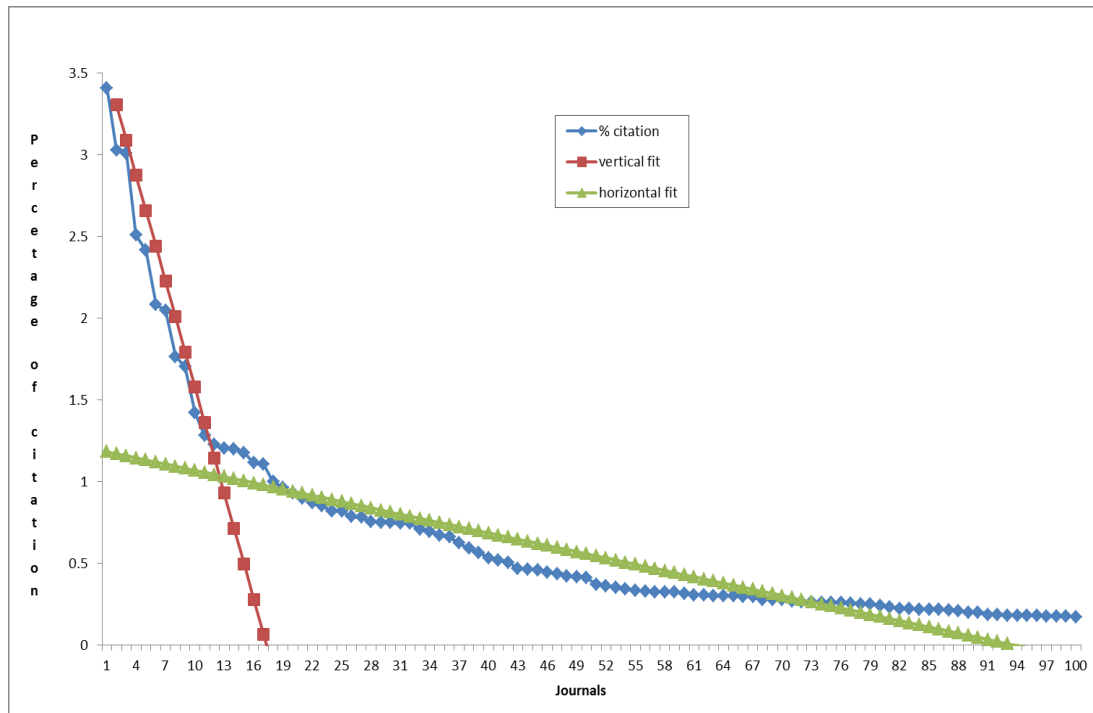
$$y = ax + b$$

$$a = \frac{n(\sum x_i y_i) - (\sum x_i)(\sum y_i)}{n(\sum x_i^2) - (\sum x_i)^2}$$

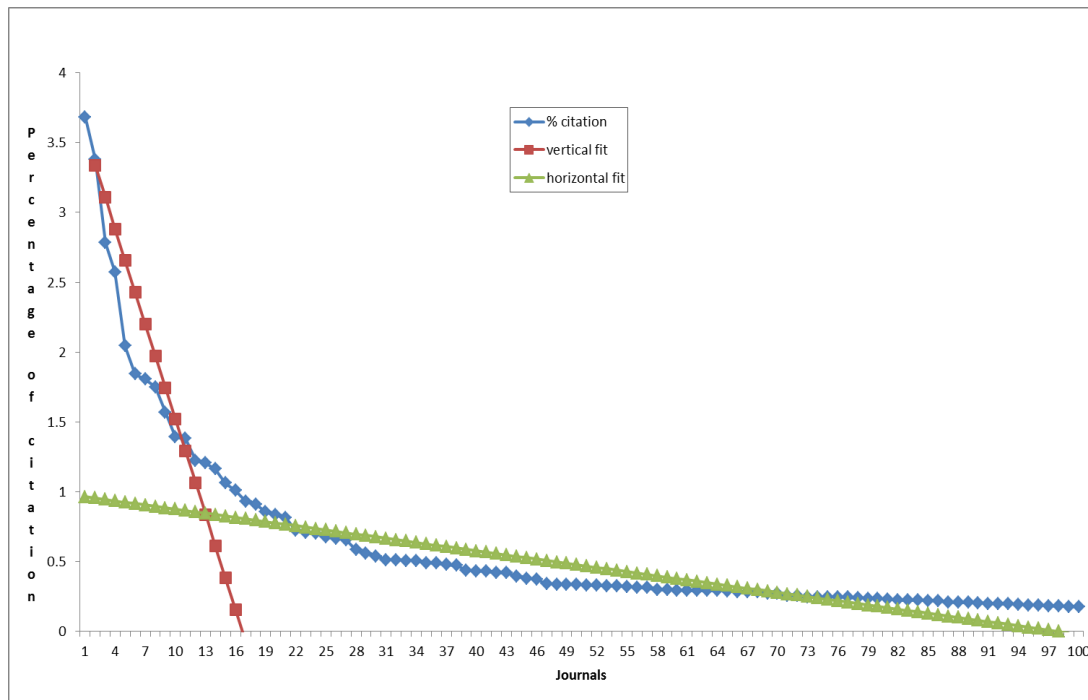
$$b = \frac{(\sum y_i) - a(\sum x_i)}{n}$$

In order to find both the location of the kink, i.e. the number of most cited journals above which the percentage of citations considerably decreases, and the slope in both subsections, we estimate a threshold kink model with an unknown threshold to approximate the curve by the two straight connected lines (Hansen, 2017) which is a modification of a structural change point (Andrews, 1993). To do that, the sum of squared residuals of both sections is minimized to determine the parameters at both sections together with the location of the kink. The journals at the right of the kink have a decreased slope, in absolute values, and, thus, contribute less to the field domain and therefore are considered as not interesting to be selected as *nano* core journals ([Figure 2](#) and [3](#)). In our analysis, the location of the kink point served

to set off 13 journals from the NST Scopus data set and 15 journals from the NTS WoS data set (Appendix 4).



**Figure 2.** Elbow criterion with threshold kink of the 100 most-cited journals from NTS Scopus data set. Red line minimizes the error between the observed and predicted value of axis y (Percentage of citation); green line minimizes the error of axis x (most cited journals)



**Figure 3.** Elbow criterion with threshold kink of the 100 most-cited journals from NST WoS data set. Red line minimizes the error between the observed and predicted value of axis y (Percentage of citation); green line minimizes the error of axis x (most cited journals)

#### *Step 4. Nano-prefix journals*

In the fourth step, we search into Scopus and WoS databases by source/publication field using the nano\* prefix for term search. All retrieved items were checked so as to choose only journals that were not ceased. By selecting only in-press journals/active journal titles in both databases (Appendix 3), we came to a total number of 91 journals. To avoid duplicates, retrieved journals with *nano* prefix in their titles that had been previously identified by the elbow criterion with threshold kink were removed from this group (3 in Scopus and 1 in WoS). A total of 88 journals were thereby selected for Scopus, and 90 for WoS.

#### *Step 5. Journal compilation from JCR and SJR plus Nano-prefix journals*

All journals contained in the NST subject category in JCR and SJR versions 2015 and 2016, excluding ceased journals, were selected. After adding the journals with *nano* prefix retrieved in step 4 to detect new journals (not identified in the previous steps), we went on to denote this group of journals

as NST A Scopus and NST B WoS. In order to avoid data duplication, the journals previously selected by employing the elbow criterion with threshold kink (step 3) were deleted from the datasets, giving 120 journals for NST A, and 123 for NST B (Appendix 5).

*Step 6. Citation analysis (from step 5)*

Publications from NST A and B were retrieved, and a separate citation analysis was accomplished. As in step 2, we determined the set of cited journals by NST A set and NST B set, as well as the number of received citations and the percentage of citations per journal. What this step aims at is to isolate prospective nuclei journals that have not been identified in the previous steps and can be identified analyzing the potential NST core journal.

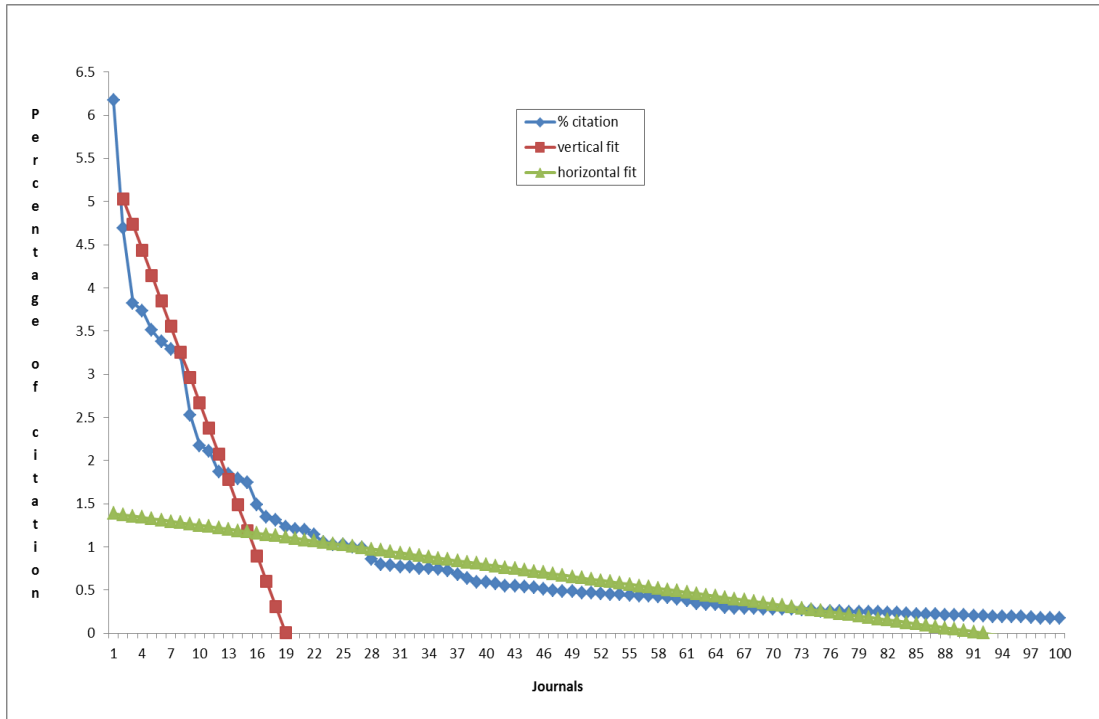
*Step 7. Elbow criterion with threshold kink (from step 6)*

Like in Step 3, the Elbow criterion with threshold kink method is used to locate the optimal kink point of the variables  $x$  and  $y$  for both sets, NST A and NST B, taking into account the 100 most cited journals by NST A set ([Figure 4](#)) and by NST B set ([Figure 5](#)). The optimal kink point predicted, in view of both data sets, is 17. All journals placed beyond point 17, including point 17, are therefore considered the nano-core journals from NST A and B (Appendix 4). Only seven previously unidentified journals from Scopus were detected, and three from WoS.

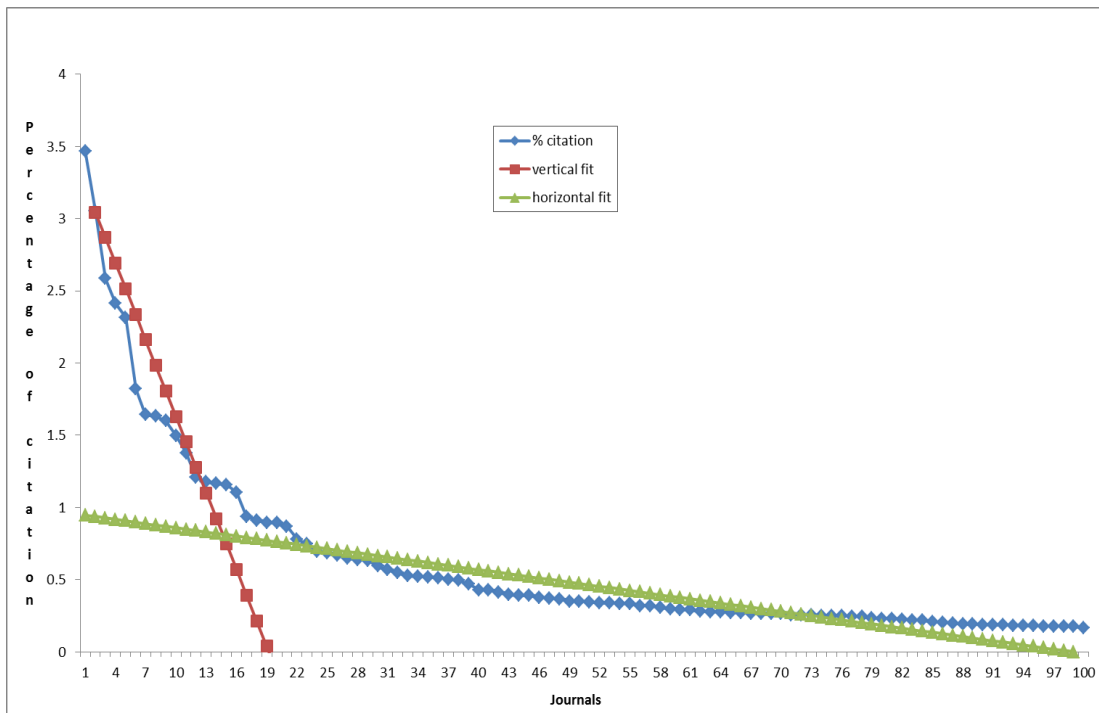
In the final step, we sum up all those journals identified throughout steps 3, 4 and 7 for each database: respectively, 108 and 110 journals<sup>5</sup> for Scopus and WoS. These two core journal lists do not show significant differences. Three journals were identified by the Scopus data set but not by WoS, and five journals were identified by WoS data yet not by Scopus. Hence, we consider the aggregation of both datasets—that is, 113 journals—to be the nano-core journals that could delineate the field of NST.

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<sup>5</sup> At first 108 were selected, but one journal had split into three different titles, for which reason all three titles were selected, making the final number of journals 110.



**Figure 4.** Elbow criterion with threshold kink of the 100 most-cited journals from NST data set A. Red line minimizes the error between the observed and predicted value of axis y (Percentage of citation); green line minimizes the error of axis x (most cited journals)



**Figure 5.** Elbow criterion with threshold kink of the 100 most-cited journals from NST data set B. Red line minimizes the error between the observed and predicted value of axis y (Percentage of citation); green line minimizes the error of axis x (most cited journals)



### 3.4. Precision and recall of the three approaches

#### 3.4.1. Precision

To compare the three approaches, we studied the precision of each at the journal level and at the publication level, following the study of Maghrebi et al. (2011). In this study, the precision is defined taking into account the definition from the National Nanotechnology Initiative of the United States (NNI): “Nanotechnology is science, engineering, and technology conducted at the nanoscale, which is about 1 to 100 nanometers. Nanoscience and nanotechnology are the study and application of extremely small things and can be used across all the other science fields, such as chemistry, biology, physics, materials science, and engineering.”<sup>6</sup>

##### 3.4.1.1. Precision by scope

In light of the “Aim and scope” and “Overview” sections, we classified journals as high, medium, or low precision based on how well they match the definition. Ultimately, we drew up the following guidelines for denoting and interpreting the results at this level:

- Value 1 = High precision. Journals that cover only NST topics
- Value 0.5 = Medium precision. Journals that cover NST topics and other topics
- Value 0 = Low precision. Journals not covering NST topics

To estimate the precision, the average of the values measured was calculated for each approach:

$$Precision (\bar{x}) = \frac{\sum_{i=1}^n x_i}{n}$$

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<sup>6</sup> <http://www.nano.gov/nanotech-101/what/definition>

#### *3.4.1.2. Precision by interviews*

We sent an online questionnaire managed by Qualtrics software to NST experts in Portugal, Spain, and The Netherlands. The experts (only Ph.D. researchers) were classified through two filters: their general background field and their particular background in NST (subfield). The questionnaire consisted of a random sample of 50 articles and reviews under different approaches and from the initial seed data: specifically, 15 articles and reviews from each approach, plus five from the seminal data (Appendix 8). Experts in NST had to indicate whether an item was relevant or not, taking into account the NNI definition. This closed question survey included a remark section per item, in case one wished to elaborate or comment on their answers. Lastly, we denoted as relevant 1 and as irrelevant 0 for the purposes of calculating precision.

#### **3.5. Recall**

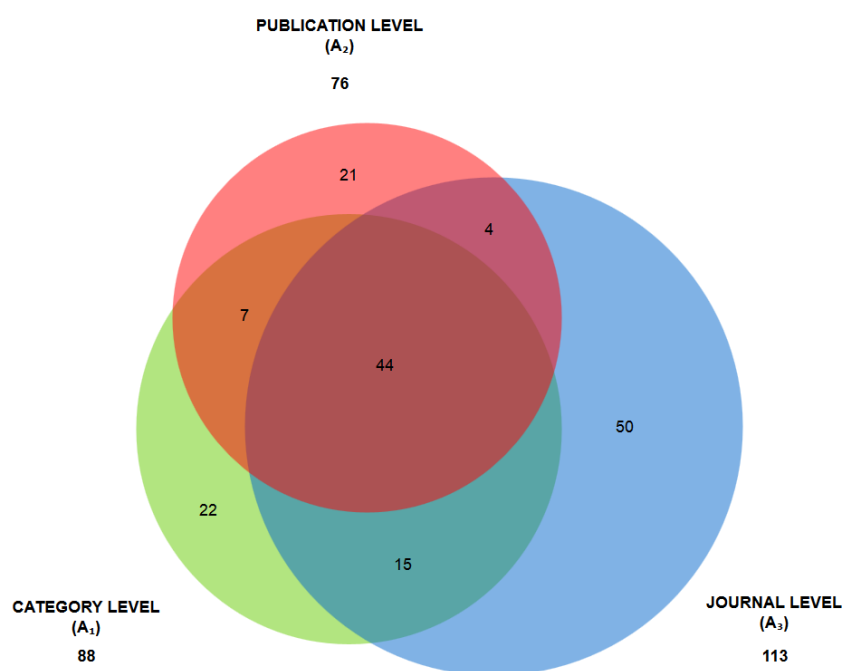
Recall, at the journal level, is derived from the assumption that the total number of journals identified by the three approaches denotes total recall, meaning total recall equals 163. In addition, we measured recall by counting journals with a high or medium level of precision. At the publication level, recall is calculated assuming that all articles and reviews identified by the three approaches should represent total recall. Thus, we considered the random sample as total recall, and considered relevant publications to be all those validated by experts whose precision was equal to or greater than 0.5.

## 4. Results

### 4.1. Comparing approaches

#### 4.1.1. Comparing approaches at the journal level ( $A_1 \cap A_2 \cap A_3$ )

The total number of journals retrieved was 163. [Figure 6](#) provides the number of journals obtained under the three approaches: 44 journals were matched by the three.



**Figure 6.** Comparison of the three approaches to delineate a field at the journal level. Numbers denote the number of journals

Altogether, 41 journals had the *nano* prefix in their titles, 22 of them covering a vast range of topics in NST, while the remaining 19 dealt only with specific NST topics (Carbon nanomaterials [1]; Nanomaterials [4]; Nanoenergy [1]; Nanoenvironment [1]; Nanomedicine and Nanobiotechnology [4]; Nanoparticles [1]; Nanophotonics [3]; Nanopatents [1]; Nanoscale communication and networking [1]; Nanotoxicology [2]). Meanwhile, three journals without the *nano* prefix covered topics related to Nanomaterials [2] and Nanochemistry [1], but were not solely related to NST (Appendix 6).

This group of journals displays a high level of precision given the fact that all topics covered by the journals are relevant in NST.

#### 4.1.2. Matching journals under two approaches

The intersection between  $A_1$  and  $A_2$  and not  $A_3$  [ $(A_1 \cap A_2) - A_3$ ] displayed seven journals; five of them focus on NST or a specific topic in NST, and the other two cover adjacent areas. As seen in Appendix 6, journals residing at this intersection may be classified under the topics: Nanomaterials; Nanoparticles; Nanophotonics; NST; Science (interdisciplinary), or Physical Chemistry.

The next intersection,  $A_1$  and  $A_3$  and not  $A_2$  [ $(A_1 \cap A_3) - A_2$ ], took in 15 journals. What is interesting here (Appendix 6) is that 13 journals shared the characteristic of the *nano* prefix in their title. In contrast, one features the prefix “micro” in its title. The journals shown in Appendix 6 cover specific areas in NST: Nanochemistry [1]; Nanoengineering [5]; Nanofluidics [1]; Nanomaterials [2]; Nanomedicine and nanobiotechnology [4]; Nanophotonics [1]; and Nanophysics [1].

The final intersection between two approaches,  $A_2 \cap A_3$  and not  $A_1$  [ $(A_2 \cap A_3) - A_1$ ], presented four journals, one of them specializing in computational nanoscience. The rest might be considered as journals that cover basic/pure knowledge applicable for research development in NST, e.g. materials science, or more specifically energy, medicine & biology, and optics & electronics.

Regarding the precision of the journals, those journals of intersection between sets  $(A_1 \cap A_2) - A_3$  and  $(A_1 \cap A_3) - A_2$  showed a high level of precision, focusing on NST. Journals in the intersection  $A_2$  with  $A_3$  and not  $A_1$  showed a lower level of precision, as they covered other knowledge fields in addition to NST-related topics.

#### 4.1.3. Journals outside the intersections

Journals that are not found to occupy any intersection are listed in Appendix 7. A<sub>1</sub> identified 22 journals outside an intersection, meaning they could only be identified under this particular approach (Appendix 7). A peculiar characteristic is shown by nine of these journals: the prefix *micro* in their titles. Although microscale studies ( $10^{-6}$ ) use a low scale, it is still larger if we take into account the definition of nanoscale ( $10^{-9}$ ). Five of these journals make reference to both scales: micro and nano; three of them make no reference to nano. Another covers a specific topic in NST, namely nanoporous materials. Besides, among the 14 remaining journals, 12 encompass *nano*-related topics, but these journals are not merely focused on *nano* research. The other two are strictly NST journals. Hence, these journals gave a high level of precision in six cases, and a medium to low level of precision in the rest.

A<sub>2</sub> detected 21 journals (Appendix 7), four focused on carbon materials, and four on electrochemistry. These electrochemistry journals may provide basic/pure knowledge for the study of nanoelectrochemistry, but they are not specialized journals in NST. Just one of them refers to NST in its scope. The same happens with two of the journals focused on condensed matter & materials physics. One focuses on the study of gold and fabricated materials. The rest of the journals identified here cover some topics close to NST or even other field categories. Six of these journals showed a high level of precision, while others displayed a medium or low level of precision.

A<sub>3</sub> distinguished 50 journals, though 31 journals are only included in the Scopus database; the other 19 journals are included in both databases (Appendix 7). Those identified journals here may be classified into two groups: journals of NST per se (general and specific) and journals connected to NST. The first group contains 34 journals on the following *nano* topics: Nanochemistry [1]; Nanoengineering [9]; Nanoenvironment [1]; Nanoethics [1]; Nanomedicine & Nanobiotechnology [7]; Nanomaterials [3]; Nanoscience

& Nanotechnology [6]; Nanoparticles [1]; Nanopharmacology [1]; and Nanotoxicology [1]. The second one contains 16 journals not specializing in an NST topic, but rather topics quite close to NST. Some of them even include the *nano* prefix or a keyword related to NST in the section 'Aim and scope', but they better match other fields of knowledge. Consequently, the precision of journals in  $A_1$  outside the intersection presented a medium to low level of precision, although the 34 journals with the *nano* prefix in their titles showed a high level of precision.

#### 4.1.4. Precision and recall at the journal level

The range of values for precision was not large. Journal approach scored the highest rank and the CWTS approach scored the lowest (Table 2). In other words, all the journals retrieved might be considered as relevant journals in NST because the values are closer to 1; just a few journals delineated by each approach might be considered non-useful journals for the delineation of NST. Recall scored lower values than precision values (Table 2). The journal approach achieved the highest values, followed by WoS category approach and CWTS. Subsequently, comparing precision and recall of the three approaches reveals a trade-off of sorts, with a slight improvement in recall for the journal approach. In sum, precision and recall performed better for the journal approach than for the WoS category and CWTS approaches, but the variation is minor.

**Table 2.** Precision and recall at the journal level

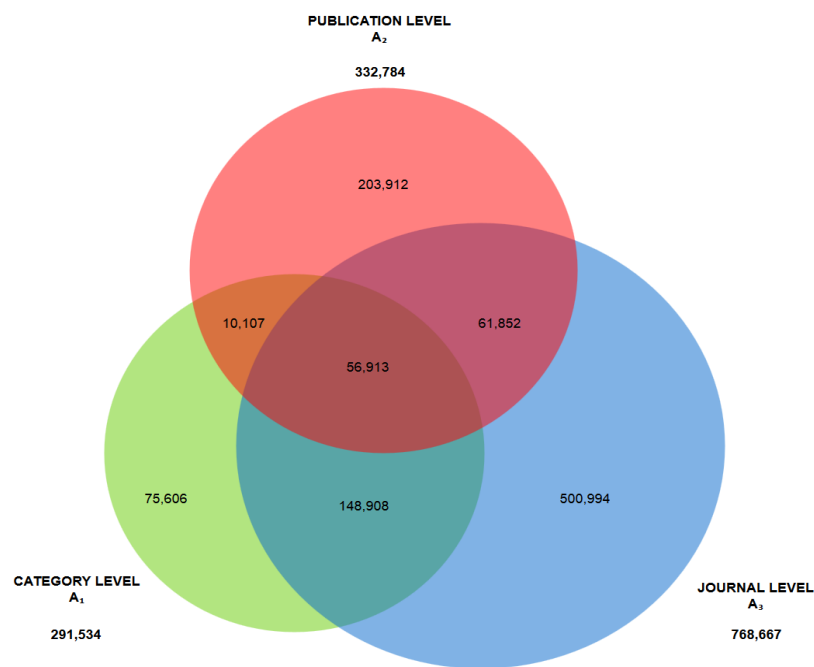
Approach	Total number of journals	Number of high-precise journals	Number of medium-precise journals	Number of low-precise journals	Precision	Recall
$A_1$	88	73	7	8	0.87	0.54
$A_2$	76	58	14	4	0.86	0.47
$A_3$	113	95	10	8	0.89	0.69

\* Total recall = 163

#### 4.2. Comparing approaches at the publication level

We use the in-house WoS database of CWTS containing 1,005,801

publications spread out in 3433 micro-level fields ( $A_0$ ). To compare the tree approaches at the publication level, all articles and reviews from 2008 to 2015 published in the covered journals by the Approach  $A_1$  and  $A_3$  were selected. For Approach  $A_2$  we use all articles and reviews from 2008 to 2015 included in micro-level fields in which at least 60% of publication overlapped with the NST initial set. [Figure 7](#) shows the number of publications identified by each approach, as well as the number of publication intersections between them.



**Figure 7.** Comparison of three approaches to delineate a field category at the publication level. Numbers denote the number of publications and reviews

#### 4.2.1. Precision at the publication level

As mentioned above, we conducted a questionnaire with a random sample to be studied by NST experts. The number of completed questionnaires was 98 (Appendix 9). According to the experts' answers, the CWTS classification approach ( $A_2$ ) achieved the top level of average precision with 0.62, followed by journal approach ( $A_3$ ) (0.56). The WoS classification approach secured the lowest value of precision (0.47) ([Table 3](#)). In addition, the seed data ( $A_0$ ) obtained 0.56 precision. Journal approach scored the highest level of recall

with a compensated precision value; WoS category approach ( $A_1$ ) displayed the same pattern. By contrast, CWTS approach, as well as the data seed, ranked high values of precision but limited recall. In other words, the higher the precision is, the lower recall is. These outcomes indicate that the journal approach may be considered an alternative approach to delineate a field, in terms of relevant publications, because of the trade-off between precision and recall.

**Table 3.** Precision and recall at publication level

Approach	Precision	Recall
$A_0$	0.56	0.38
$A_1$	0.47	0.34
$A_2$	0.62	0.34
$A_3$	0.56	0.46

Most of the questionnaires were completed by physicists, chemists, biologists and engineers. Taking into account the background field of each interviewee (Appendix 10), all fields, except materials science, considered that the approach with the highest level of precision was CWTS, closely followed by the journal approach.

The comparison of precision outcomes at the publication level and at the journal level showed distinctions. Precision at journal level identified the journal approach as the most precise, although there is no significant difference with regard to the other approaches. Nevertheless, precision at the publication level ranked CWTS classification as the most precise approach. It so happens that many journals publish *nano* publications, but at the same time, they continue to put out publications close to *nano* yet not specifically NST. This could be why there is a distinction when comparing the two approaches: studying precision at the publication level, we see it in greater detail, allowing for a more objective assessment of precision.



In general, a very substantial level of disagreement was detected in terms of the background field of each interviewee and the perceived relevance or irrelevance of an item according to the responses. We should point out that no publication received a 100% answer as relevant or not according to the experts.

In order to analyze/evaluate the level/reliability of agreement among experts, we used Fleiss's kappa statistic (Fleiss, 1971) for interrater reliability. This value ranges from -1 to +1, where 0 represents agreement expected at random and 1 represents perfect agreement among experts. In addition, we used the Landis and Koch (1977) guidelines for interpreting Fleiss's kappa values. The resulting level/reliability of agreement among all experts was 0.27 (Table 4). Some disagreement among the experts might be traced to their different backgrounds, hence their beliefs about what is relevant or not in the field.

**Table 4.** Fleiss's Kappa values

	Fleiss's kappa
<b>Total</b>	0.27

Field	Fleiss's kappa
Physics	0.31
Chemistry	0.26
Engineering	0.18
Biology	0.09

Subfield	Fleiss's kappa
Nanotheoretical physics	0.42
Nanobiosystems	0.40
Nanomagnetism	0.34
Nanoelectronics	0.29
Nanomaterials	0.26
Nanobiomedicine	0.24
Nanoprocesses	0.21
Nanoenergy	0.19
Nanoengineering	0.19
Nanophotonics	0.19
Nanotoxicology & Sustainability	0.16
Nanofabrication	0.07

Despite the fact that the random sample involved different approaches, publications with a 0.8 of precision or more were selected, 13 publications in

total. After matching these publications to the three approaches, the journal approach was found to match 10 publications (76.92%) and CWTS classification approach matched seven (53.84%). This could mean that although the average of precision in the journal approach is less than under the CWTS classification, there are many relevant publications in the journal approach. For example, three of the four publications with 0.9 (or over) percentage of precision match the journal approach; only once matches the CWTS classification approach.

The results obtained after the validation process by experts determined whether journal publications were relevant or not relevant. In view of the validation process, it was unexpectedly found that journals putting out relevant publications also put out irrelevant publications. It may be that many publications tend to be classified as *nano* publications, but they are not NST per se. Our random sample set is too small to compare results at the journal level, that is, taking into account journal title, with the journal included in the sample.

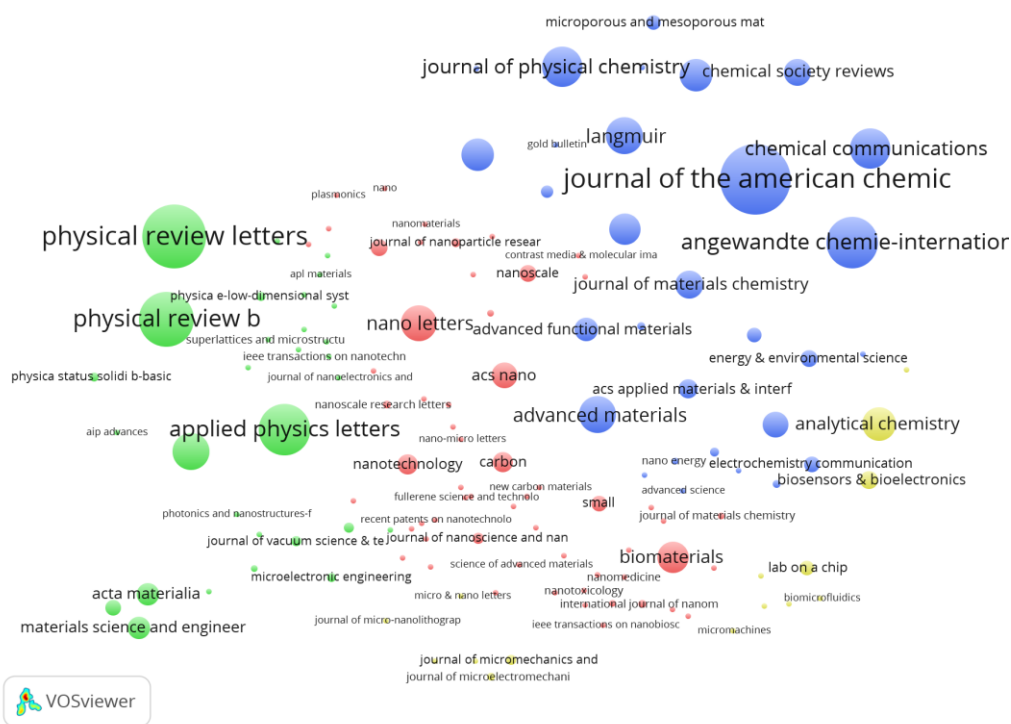
#### *4.3. Visualization maps at the publication level*

Visualization of the data was achieved through VOSviewer software (van Eck & Waltman, 2010) and shows the journals in the field of NST under the three approaches ([Figure 8](#)). The journals were clustered by using co-citation analysis. The map is based on co-citation data. The co-citation frequency of NST core journals was determined based on citations in articles and reviews published from 2008-2016 to articles published in NST journals from 2008 to 2015. In overlay visualizations, the maps show the distribution of publications across the NST core journals map. The overlap indicates the inclusion of a journal that belongs to a particular approach in the NST core journals map.

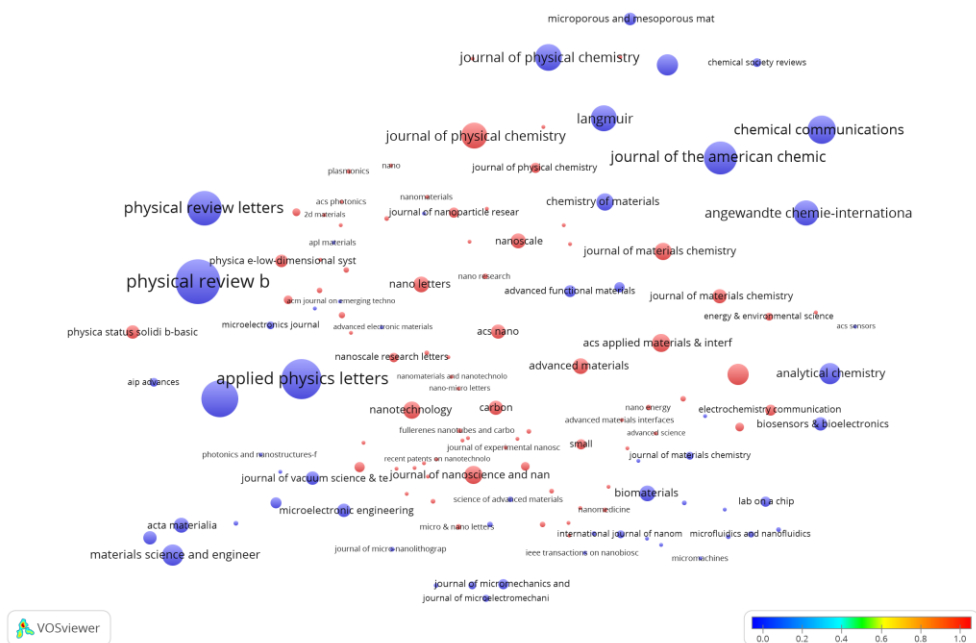
Each circle represents a journal. The size of each journal represents the number of citations received. Journals located close to each other are more related than journals located far away. Color indicates that clusters, as well as

journals in each cluster, are strongly related to each other. Four clusters are seen, three of them large and one small. The group of journals for every cluster can be summed up as: journals focusing on physics in the middle and lower left (green); journals focusing on areas in NST in the middle (red); journals focusing on chemistry toward the upper and middle right; and journals focusing on micro and nanoengineering to the lower right (yellow).

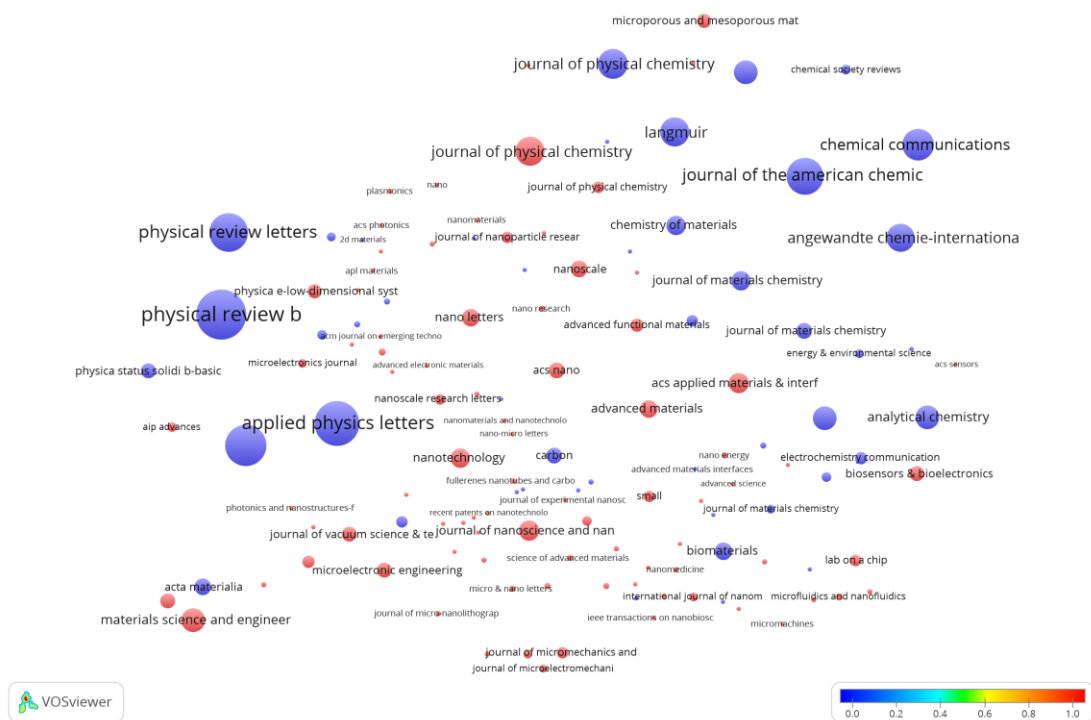
The red cluster consists of journals that publish the scientific output in NST, covering journals publishing all areas of NST, and nanomaterials-physical and mechanical characteristics (upper middle) and nanomaterials-structure and properties (lower middle). The green cluster holds journals publishing nanophysics research, although journals on physics are included as well. The lower area of this cluster displays journals focusing on micro and nanoengineering process (the physics, engineering, and materials of the devices). The blue one consists of journals on chemistry research. Lastly, the yellow cluster consists of journals focused on micro and nanoengineering, but applied to biology, medicine, and chemistry.



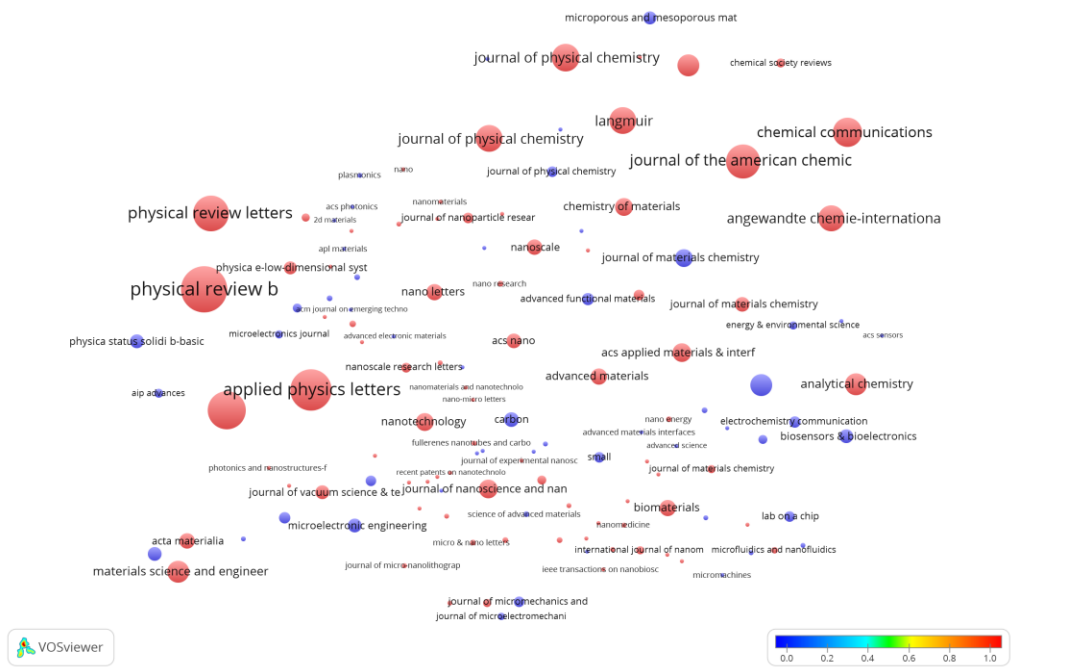
**Figure 8.** NST journals citation network



**Figure 9.** Overlap map of number of publications per journal by CWTS approach ( $A_2$ )



**Figure 10.** Overlap map of number of publications per journal by WoS approach ( $A_1$ )



**Figure 11.** Overlap map of number of publications per journal by journal approach ( $A_3$ )

Overlapped visualization based on a number of publications by the journal in each approach illustrates that most journals with a high level of overlap in  $A_2$  are located in the middle area, and no many of them are in the outer periphery ([Figure 9](#)). In a similar vein, many of the journals from  $A_1$  are located in the middle area, although many others are in the outer periphery ([Figure 10](#)). By contrast, journals from  $A_3$  are located all over the visualization ([Figure 11](#)). As is clearly seen, many of the journals distinguished by this approach are located in the outer area, and many of the journals located in the middle areas are not selected by this approach ( $A_3$ ). That is, many of the journal located in middle areas of the map are not been identified by the journal approach ( $A_3$ ). Instead, they have been identified by the use of approaches  $A_1$  or  $A_2$ .

## **5. Discussion and Conclusions**

The overall advancement of research means that new fields are emerging, and they may be hard to define. Yet proper field delineation is essential for information retrieval purposes and designing reliable and solid tools, especially in the framework of science policy design and science evaluation processes. In this paper, we deal with the problem that researchers face when attempting to delineate emergent and interdisciplinary fields such as NST.

Evidence shows that the use of different multidisciplinary and international bibliographical data sources —such as Scopus and WoS— for collecting data and comparing approaches can contribute to accurate field delineation (Glänzel, 2015), although the completeness and quality of the data set might be skewed (Mongeon & Paul-Hus, 2016). Nevertheless, a systematic framework to harvest the scientific production of a field by the enrichment of new terminology, specialized journals and citation analysis can help in defining a precise data collection (Huang et al., 2015). The inexistence, thus far, of an international gold-standard classification system for bibliometric fields has been underlined in previous studies (Gómez et al., 1996; Waltman & van Eck, 2012). It is well known that field delineation is problematic, even

when different data sources are used, new methods are applied, citation relations are measured, precision and recall are calculated, and the results are validated by experts. While validation by experts in the field may enhance the quality of the delineation process, a lack of agreement may prevail, with opinions partly conditioned by the experts' particular field of work.

Depending on the field to be delineated and the purpose at hand, each of the methods suggested in this study could be suitable (Zitt, 2015). All the approaches have their pros and cons. Each vision reflects nuances that contribute to field delineation in some way or another. Because no method can be singled out as the best one, this study aimed to contribute empirically to the questionable area of using search strategies and citation analysis at the journal level to delineate research fields. Key elements for the success of such a process are the application and replicability of methods used, and the design and development of classifications, indicators and/or tools relying on scientific references from databases. A comparative and reproducible method is essential for arriving at consistent and reliable results. The approach presented here entails a seven-step procedure that can be transferred and replicated in other research areas and emergent fields in large databases characterized by a very robust and detailed framework to observe the coverage of a field depending on which method has been applied. The application of these approaches in NST field or in any field of knowledge at different levels of aggregation may suggest significant implications for understanding how the diversity of the outcomes might help to improve them. Depending on the approach or the different actors (countries, institutions, etc.) used, a combination of results may provide some support for the delineation of accurate fields. This is evident in the case of country analysis where a bigger or lower number of country journals or publications can be analyzed in accordance with the approach utilized (Wang et al., 2019).

Our line of research has become a series of stepping-stones (Gómez-Núñez et al., 2011; Gómez-Núñez et al., 2014; Muñoz-Écija et al., 2013) toward the

goal of optimizing and boosting the SJR journal classification system and subsequent journal assignment. In this study itself, taking journals as units of analysis did not guarantee proper identification of the publications: some publications belonged to other subject categories, some journals that had published relevant output in the field were not included under the corresponding subject category, etc. Notwithstanding, the journal classification system can be said to display “a robust poor health”. It is still used by the main bibliographical databases such as Scopus and WoS. The classifications are of widespread interest and utility when it comes to evaluating science and research, and a valuable resource for decision- and policy-makers (e.g., when hiring, promoting and funding research assessment exercises). We do not proclaim that this classification proposal is definitive or exclusively appropriate. Rather, within the context of classifying emerging and interdisciplinary fields like NST, we conclude it is necessary to keep striving to combine techniques and units of analysis in the search for a process that will lead us closer to consensus among the scientific community.

### **Limitations and future research**

It is assumed that the compiled search suggested in this work should be continuously updated because of NST shift to new research lines. For example, the keyword *silicene* has not been included in any NST lexical queries when this study was conducted. However, it can be deemed as a prospective term to add in future lexical queries (Wang et al., 2019).

Despite the fact that extrapolations of the approach at journal level may be conducted to other fields, it could contemplate the omission of Steps 6 and 7. These steps aim to isolate prospective nuclei journals that have not emerged in previous steps of the method. This study has shown that only a few journals have been identified by Step 7. Surprisingly, many of them are not NST core journals in terms precision and recall (Appendix 11). It can therefore be assumed that researchers may decide optionally the usefulness of these steps when they apply this methodology to delineate other fields of



knowledge. They may take into account whether they perform the steps or not, and whether they select all journals or only the most cited ones.

Finally, a sample based on publications for designing the online questionnaire was used in this study, but sample-based on journals could have been considered instead. In any case, to guarantee a high response rate from interviewees, both random sample-based on publications or on journals should be considered determining features of the online survey to guarantee a high response rate from interviewees (Holbrook et al., 2006; Ganassali, 2008; Galesic & Bosnjak, 2009; M. Liu & Wronski, 2017).

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### **Author's contribution**

**Teresa Muñoz-Écija:** Conceived and designed the analysis; Collected the data; Contributed data or analysis tools; Performed the analysis; Wrote the paper.

**Benjamín Vargas-Quesada:** Contributed data or analysis tools; Wrote the paper.

**Zaida Chinchilla-Rodríguez:** Conceived and designed the analysis; Wrote the paper.

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## Appendix A. Supplementary data

### Appendix 1a. Journals list of WoS category Nanoscience & Nanotechnology (ceased journals excluded)

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<i>Journals list of WoS category N&amp;N</i>
ACM JOURNAL ON EMERGING TECHNOLOGIES IN COMPUTING SYSTEMS
ACS APPLIED MATERIALS & INTERFACES
ACS ENERGY LETTERS
ACS NANO
ACS PHOTONICS
ACS SENSORS
ADVANCED ELECTRONIC MATERIALS
ADVANCED FUNCTIONAL MATERIALS
ADVANCED HEALTHCARE MATERIALS
ADVANCED MATERIALS
ADVANCED SCIENCE
ADVANCES IN NATURAL SCIENCES-NANOSCIENCE AND NANOTECHNOLOGY
AIP ADVANCES
APL MATERIALS
APPLIED NANOSCIENCE
BEILSTEIN JOURNAL OF NANOTECHNOLOGY
BIOMEDICAL MICRODEVICES
BIOMICROFLUIDICS
BIOSENSORS & BIOELECTRONICS
CHEMNANOMAT
CURRENT NANOSCIENCE
DIGEST JOURNAL OF NANOMATERIALS AND BIOSTRUCTURES
ENVIRONMENTAL SCIENCE-NANO
FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES
IEEE TRANSACTIONS ON NANOBIOSCIENCE
IEEE TRANSACTIONS ON NANOTECHNOLOGY
IET NANOBIO TECHNOLOGY
INORGANIC AND NANO-METAL CHEMISTRY
INTERNATIONAL JOURNAL OF NANOMEDICINE
INTERNATIONAL JOURNAL OF NANOTECHNOLOGY
JOURNAL OF BIOMEDICAL NANOTECHNOLOGY
JOURNAL OF EXPERIMENTAL NANOSCIENCE
JOURNAL OF LASER MICRO NANOENGINEERING
JOURNAL OF MICROELECTROMECHANICAL SYSTEMS
JOURNAL OF MICROMECHANICS AND MICROENGINEERING
JOURNAL OF MICRO-NANOLITHOGRAPHY MEMS AND MOEMS
JOURNAL OF NANO RESEARCH
JOURNAL OF NANOBIO TECHNOLOGY

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*Journals list of WoS category N&N*

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JOURNAL OF NANOELECTRONICS AND OPTOELECTRONICS

JOURNAL OF NANOMATERIALS

JOURNAL OF NANOPARTICLE RESEARCH

JOURNAL OF NANOPHOTONICS

JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY

JOURNAL OF PHYSICAL CHEMISTRY C

JOURNAL OF PHYSICAL CHEMISTRY LETTERS

JOURNAL OF VACUUM SCIENCE & TECHNOLOGY B

LAB ON A CHIP

MATERIALS EXPRESS

MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING

MICRO & NANO LETTERS

MICROELECTRONIC ENGINEERING

MICROELECTRONICS JOURNAL

MICROELECTRONICS RELIABILITY

MICROFLUIDICS AND NANOFUIDICS

MICROMACHINES

MICROPOROUS AND MESOPOROUS MATERIALS

MICROSYSTEM TECHNOLOGIES-MICRO-AND NANOSYSTEMS-INFORMATION STORAGE AND PROCESSING SYSTEMS

NANO

NANO COMMUNICATION NETWORKS

NANO ENERGY

NANO LETTERS

NANO RESEARCH

NANO TODAY

NANOMATERIALS

NANOMATERIALS AND NANOTECHNOLOGY

NANOMEDICINE

NANOMEDICINE-NANOTECHNOLOGY BIOLOGY AND MEDICINE

NANO-MICRO LETTERS

NANOPHOTONICS

NANOSCALE

NANOSCALE AND MICROSCALE THERMOPHYSICAL ENGINEERING

NANOSCALE RESEARCH LETTERS

NANOSCIENCE AND NANOTECHNOLOGY LETTERS

NANOTECHNOLOGY

NANOTECHNOLOGY REVIEWS

NANOTOXICOLOGY

NATURE NANOTECHNOLOGY

PARTICLE & PARTICLE SYSTEMS CHARACTERIZATION

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*Journals list of WoS category N&N*

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PHOTONICS AND NANOSTRUCTURES-FUNDAMENTALS AND APPLICATIONS

PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES

PLASMONICS

PRECISION ENGINEERING-JOURNAL OF THE INTERNATIONAL SOCIETIES FOR PRECISION ENGINEERING AND NANOTECHNOLOGY

RECENT PATENTS ON NANOTECHNOLOGY

REVIEWS ON ADVANCED MATERIALS SCIENCE

SCIENCE OF ADVANCED MATERIALS

SCRIPTA MATERIALIA

SMALL

WILEY INTERDISCIPLINARY REVIEWS-NANOMEDICINE AND NANOBIO TECHNOLOGY

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**Appendix 1b. Journals list of SJR category Nanoscience & Nanotechnology  
(ceased and discontinued published journals excluded)**

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ACM JOURNAL ON EMERGING TECHNOLOGIES IN COMPUTING SYSTEMS

ACS APPLIED MATERIALS & INTERFACES

ACS NANO

ADVANCED FUNCTIONAL MATERIALS

ADVANCED MATERIALS

AIP ADVANCES

BEILSTEIN JOURNAL OF NANOTECHNOLOGY

BIOMATERIALS

BIOMEDICAL MICRODEVICES

BIOMICROFLUIDICS

BIOSENSORS AND BIOELECTRONICS

CURRENT NANOSCIENCE

DIGEST JOURNAL OF NANOMATERIALS AND BIOSTRUCTURES

E-JOURNAL OF SURFACE SCIENCE AND NANOTECHNOLOGY

FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES

IEEE NANOTECHNOLOGY MAGAZINE

IEEE TRANSACTIONS ON NANOBIO SCIENCE

IEEE TRANSACTIONS ON NANOTECHNOLOGY

IET NANOBIO TECHNOLOGY

INTERNATIONAL JOURNAL OF NANO AND BIOMATERIALS

INTERNATIONAL JOURNAL OF NANOMANUFACTURING

INTERNATIONAL JOURNAL OF NANOMECHANICS SCIENCE AND TECHNOLOGY

INTERNATIONAL JOURNAL OF NANOMEDICINE

INTERNATIONAL JOURNAL OF NANOPARTICLES

INTERNATIONAL JOURNAL OF NANOSCIENCE

INTERNATIONAL JOURNAL OF NANOTECHNOLOGY

JOURNAL OF BIOMEDICAL NANOTECHNOLOGY

JOURNAL OF BIONANOSCIENCE

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JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE

JOURNAL OF EXPERIMENTAL NANOSCIENCE

JOURNAL OF LASER MICRO NANOENGINEERING

JOURNAL OF MICRO/ NANOLITHOGRAPHY, MEMS, AND MOEMS

JOURNAL OF MICROMECHANICS AND MICROENGINEERING

JOURNAL OF MICRO-BIO ROBOTIC

JOURNAL OF NANO RESEARCH

JOURNAL OF NANOBIO TECHNOLOGY

JOURNAL OF NANO ELECTRONICS AND OPTOELECTRONICS

JOURNAL OF NANOMATERIALS

JOURNAL OF NANOPARTICLE RESEARCH

JOURNAL OF NANOPHOTONICS

JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY

JOURNAL OF PHYSICAL CHEMISTRY C

JOURNAL OF PHYSICAL CHEMISTRY LETTERS

JOURNAL OF SURFACE INVESTIGATION

LAB ON A CHIP - MINIATURISATION FOR CHEMISTRY AND BIOLOGY

MATERIALS EXPRESS

MATERIALS SCIENCE & ENGINEERING A: STRUCTURAL MATERIALS: PROPERTIES, MICROSTRUCTURE AND PROCESSING

MICRO AND NANO LETTERS

MICRO AND NANOSYSTEMS

MICROELECTRONIC ENGINEERING

MICROELECTRONICS AND RELIABILITY

MICROELECTRONICS JOURNAL

MICROFLUIDICS AND NANOFUIDICS

MICROPOROUS AND MESOPOROUS MATERIALS

MICROSYSTEM TECHNOLOGIES

NAMI JISHU YU JINGMI GONGCHENG/NANOTECHNOLOGY AND PRECISION ENGINEERING

NANO

NANO BIOMEDICINE AND ENGINEERING

NANO LETTERS

NANO RESEARCH

NANO TODAY

NANOETHICS

NANOMEDICINE

NANOMEDICINE: NANOTECHNOLOGY, BIOLOGY, AND MEDICINE

NANO-MICRO LETTERS

NANOSCALE

NANOSCALE RESEARCH LETTERS

NANOSCIENCE AND NANOTECHNOLOGY - ASIA

NANOSCIENCE AND NANOTECHNOLOGY LETTERS

NANOTECHNOLOGIES IN RUSSIA

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**NANOTECHNOLOGY**

**NANOTECHNOLOGY PERCEPTIONS**

**NANOTECHNOLOGY, SCIENCE AND APPLICATIONS**

**NANOTOXICOLOGY**

**NATURE NANOTECHNOLOGY**

**PHOTONICS AND NANOSTRUCTURES - FUNDAMENTALS AND APPLICATIONS**

**PHYSICA E: LOW-DIMENSIONAL SYSTEMS AND NANOSTRUCTURES**

**PLASMONICS**

**PRECISION ENGINEERING**

**PROCEEDINGS OF THE INSTITUTION OF MECHANICAL ENGINEERS, PART N: JOURNAL OF NANOMATERIALS, NANOENGINEERING AND NANOSYSTEMS**

**RECENT PATENTS ON NANOTECHNOLOGY**

**REVIEWS ON ADVANCED MATERIALS SCIENCE**

**SCIENCE OF ADVANCED MATERIALS**

**SCRIPTA MATERIALIA**

**SMALL**

**WILEY INTERDISCIPLINARY REVIEWS NANOMEDICINE AND NANOBIO TECHNOLOGY**

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## **Appendix 2. Lexical queries for Scopus and WoS**

### **Lexical queries for Scopus**

#1

TITLE-ABS-KEY(nano\* )

#2

(TITLE-ABS-KEY ( nanoa ) OR TITLE-ABS-KEY ( nanoacalles ) OR TITLE-ABS-KEY ( nanoagraylea ) OR TITLE-ABS-KEY ( nanoalga\* ) OR TITLE-ABS-KEY ( nanoapiculatum ) OR TITLE-ABS-KEY ( nanoarchaeaor ) OR TITLE-ABS-KEY ( nanoarchaeota ) OR TITLE-ABS-KEY ( nanoarchaeum ) OR TITLE-ABS-KEY ( nanoastegotherium ) OR TITLE-ABS-KEY ( "nano\*aryote\*" ) OR TITLE-ABS-KEY ( nanobacteri\* ) OR TITLE-ABS-KEY ( nanobagrus ) OR TITLE-ABS-KEY ( nanobalcis ) OR TITLE-ABS-KEY ( nanobaris ) OR TITLE-ABS-KEY ( nanobates ) OR TITLE-ABS-KEY ( nanobatinae ) OR TITLE-ABS-KEY ( nanobius ) OR TITLE-ABS-KEY ( nanobryaceae ) OR TITLE-ABS-KEY ( nanobryoides ) OR TITLE-ABS-KEY ( nanobuthus ) OR TITLE-ABS-KEY ( nano-bible ) OR TITLE-ABS-KEY ( nanocalcar ) OR TITLE-ABS-KEY ( nanocambridgea ) OR TITLE-ABS-KEY ( nanocapillare ) OR TITLE-ABS-KEY ( nanocapillary ) OR TITLE-ABS-KEY ( nanocarpa ) OR TITLE-ABS-KEY ( nanocarpum ) OR TITLE-ABS-KEY ( nanocarpus ) OR TITLE-ABS-KEY ( nanocassiope ) OR TITLE-ABS-KEY ( nanocavia ) OR TITLE-ABS-KEY ( nanocephalum ) OR TITLE-ABS-KEY ( nanocheirodon ))

#3

(TITLE-ABS-KEY ( nanochilina ) OR TITLE-ABS-KEY ( nanochilus ) OR TITLE-ABS-KEY ( nanochitina ) OR TITLE-ABS-KEY ( nanochlaenius ) OR TITLE-ABS-KEY ( nanochlorum ) OR TITLE-ABS-KEY ( nanochoerus ) OR TITLE-ABS-KEY ( nanochromis ) OR TITLE-ABS-KEY ( nanochromosom\* ) OR TITLE-ABS-KEY ( nanochrysopa ) OR TITLE-ABS-KEY ( nanochthonius ) OR TITLE-ABS-KEY ( nanocixius ) OR TITLE-ABS-KEY ( nanocladus ) OR TITLE-ABS-KEY ( nanoclarella ) OR TITLE-ABS-KEY ( nanoclavelia ) OR TITLE-ABS-KEY ( nanoclimacium ) OR TITLE-ABS-KEY ( nanoclymenia ) OR TITLE-ABS-KEY ( nanocnide ) OR TITLE-ABS-KEY ( nanocochlea ) OR TITLE-ABS-KEY ( nanocolletes ) OR TITLE-ABS-KEY ( nanocondylodesmus ) OR TITLE-ABS-KEY ( nanocopia ) OR TITLE-ABS-KEY ( nanocoquimba ) OR TITLE-ABS-KEY ( nanocrinus ) OR TITLE-ABS-KEY ( nanoctenus ) OR TITLE-ABS-KEY ( nanocthispa ) OR TITLE-ABS-KEY ( nanocuridae ) OR TITLE-ABS-KEY ( nanocurie ) OR TITLE-ABS-KEY ( nano-curie ) OR TITLE-ABS-KEY ( nanocuris ) OR TITLE-ABS-KEY ( nanocyclopia ) OR TITLE-ABS-KEY ( nanocynodon ) OR TITLE-ABS-KEY ( nanocythere ))

#4

(TITLE-ABS-KEY ( nanodacna ) OR TITLE-ABS-KEY ( nanodactylus ) OR TITLE-ABS-KEY ( nanodamon ) OR TITLE-ABS-KEY ( nanodea ) OR TITLE-ABS-KEY ( nanodealbata ) OR TITLE-ABS-KEY ( nanodectes ) OR TITLE-ABS-KEY ( nanodella ) OR TITLE-ABS-KEY ( nanodelphys ) OR TITLE-ABS-KEY ( nanodendron ) OR TITLE-ABS-KEY ( nanodes ) OR TITLE-ABS-KEY ( nanodiaparsis ) OR TITLE-ABS-KEY ( nanodiaptomus ) OR TITLE-ABS-KEY ( nanodidelphys ) OR TITLE-ABS-KEY ( nanodiella ) OR TITLE-ABS-KEY ( nanodiodes ) OR TITLE-ABS-KEY ( nanodiplois ) OR TITLE-ABS-KEY ( nanodiscus ) OR TITLE-ABS-KEY ( nanodisticha ) OR TITLE-ABS-KEY ( nanodromia ) OR TITLE-ABS-KEY ( nanodynerus ) OR TITLE-ABS-KEY ( nanoesi ) OR TITLE-ABS-KEY ( nanofauna\* ) OR TITLE-ABS-KEY ( nanofila ) OR TITLE-ABS-KEY ( "nano-filt\*" ) OR TITLE-ABS-KEY ( nanofilt\* ) OR TITLE-ABS-KEY ( nanoflagel\* ) OR TITLE-ABS-KEY ( nanoflow ) OR TITLE-ABS-KEY ( "nano-flow" ) OR TITLE-ABS-KEY ( nanofilidae ) OR TITLE-ABS-KEY( Nanog ) OR TITLE-ABS-KEY( Nanog1 ))

#5

(TITLE-ABS-KEY( Nanog2 ) OR TITLE-ABS-KEY( Nanogalatea ) OR TITLE-ABS-KEY( Nanogeterotroph\* ) OR TITLE-ABS-KEY( Nanoglobum ) OR TITLE-ABS-KEY( Nanoglossa ) OR TITLE-ABS-KEY( Nanognathia ) OR TITLE-ABS-KEY( Nanognathus ) OR TITLE-ABS-KEY( Nanogomphodon ) OR TITLE-ABS-KEY( Nanogona ) OR TITLE-ABS-KEY( Nanogonalos ) OR TITLE-ABS-KEY( Nanogorgon ) OR TITLE-ABS-KEY( Nanogram\* ) OR TITLE-ABS-KEY("nano-gram\*" ) OR TITLE-ABS-KEY( Nanogramma ) OR TITLE-ABS-KEY( Nanograptus ) OR TITLE-ABS-KEY( Nanogyra ) OR TITLE-ABS-KEY( Nanogyrini ) OR TITLE-ABS-KEY(

Nanohalus ) OR TITLE-ABS-KEY( Nanohammus ) OR TITLE-ABS-KEY( Nanohemicera ) OR TITLE-ABS-KEY( Nanoheterotroph\* ) OR TITLE-ABS-KEY( Nanohystrix ) OR TITLE-ABS-KEY( Nanoides ) OR TITLE-ABS-KEY( Nanoini ) OR TITLE-ABS-KEY( Nanojapyx ) OR TITLE-ABS-KEY( Nanokerala ) OR TITLE-ABS-KEY( Nanokelvin\* ) OR TITLE-ABS-KEY( Nanokermes ) OR TITLE-ABS-KEY( Nanola ) OR TITLE-ABS-KEY( Nanolachesilla ) OR TITLE-ABS-KEY( Nanolania ) OR TITLE-ABS-KEY( Nanolauthia ) OR TITLE-ABS-KEY( NanoLC\* ) OR TITLE-ABS-KEY("nano-LC\*" ) OR TITLE-ABS-KEY( Nanolestes ) OR TITLE-ABS-KEY( Nanolichus ) OR TITLE-ABS-KEY("nano-liter\*" ) OR TITLE-ABS-KEY("nano-litre\*" ) OR TITLE-ABS-KEY( Nanoliter\* ) OR TITLE-ABS-KEY( Nanolitre\* ) OR TITLE-ABS-KEY( Nanolobus ) OR TITLE-ABS-KEY( Nanoloricida ))

#6

(TITLE-ABS-KEY( Nanolpium ) OR TITLE-ABS-KEY( Nanolumen ) OR TITLE-ABS-KEY( Nanomaja ) OR TITLE-ABS-KEY( Nanomantinae ) OR TITLE-ABS-KEY( Nanomantini ) OR TITLE-ABS-KEY( Nanomantis ) OR TITLE-ABS-KEY( Nanomeli\* ) OR TITLE-ABS-KEY( Nanomelon ) OR TITLE-ABS-KEY( Nanomermis ) OR TITLE-ABS-KEY( Nanomerus ) OR TITLE-ABS-KEY( Nanomeryx ) OR TITLE-ABS-KEY( Nanometa ) OR TITLE-ABS-KEY("nano-meter\*" ) OR TITLE-ABS-KEY( Nanometidae ) OR TITLE-ABS-KEY( Nanometinae ) OR TITLE-ABS-KEY( Nanometra ) OR TITLE-ABS-KEY("nano-metre\*" ) OR TITLE-ABS-KEY("nm" ) OR TITLE-ABS-KEY( Nanometer\* ) OR TITLE-ABS-KEY( Nanometre\* ) OR TITLE-ABS-KEY( Nanomia ) OR TITLE-ABS-KEY( Nanomias ) OR TITLE-ABS-KEY( Nanomicrophyes ) OR TITLE-ABS-KEY( Nanomilleretta ) OR TITLE-ABS-KEY( Nanomimus ) OR TITLE-ABS-KEY( Nanomis ) OR TITLE-ABS-KEY( Nanomitra ) OR TITLE-ABS-KEY( Nanomitriella ) OR TITLE-ABS-KEY( Nanomitriopsis ) OR TITLE-ABS-KEY( Nanomitus ) OR TITLE-ABS-KEY( Nanomol\* ) OR TITLE-ABS-KEY("nano-molar" ) OR TITLE-ABS-KEY("nano-mole\*" ) OR TITLE-ABS-KEY( Nanomutilinae ) OR TITLE-ABS-KEY( Nanomutilla ) OR TITLE-ABS-KEY( Nanomyces ) OR TITLE-ABS-KEY( Nanomyina ) OR TITLE-ABS-KEY( Nanomyrmacyba ) OR TITLE-ABS-KEY( Nanomyrme ) OR TITLE-ABS-KEY( Nanomys ) OR TITLE-ABS-KEY( Nanomysis ) OR TITLE-ABS-KEY( Nanomysmena ))

#7

(TITLE-ABS-KEY( Nanonaucoris ) OR TITLE-ABS-KEY( Nanonavis ) OR TITLE-ABS-KEY( Nanoneis ) OR TITLE-ABS-KEY( Nanonemoura ) OR TITLE-ABS-KEY( Nanonocticolus ) OR TITLE-ABS-KEY( Nanonycteris ) OR TITLE-ABS-KEY("Nanook of the North" ) OR TITLE-ABS-KEY ( nanopachyiulus ) OR TITLE-ABS-KEY ( nanopagurus ) OR TITLE-ABS-KEY ( nanopareia ) OR TITLE-ABS-KEY ( nanoparia ) OR TITLE-ABS-KEY ( nanopatula ) OR TITLE-ABS-KEY ( nanopennatum ) OR TITLE-ABS-KEY ( nanoperla ) OR TITLE-ABS-KEY ( nanophareus ) OR TITLE-ABS-KEY ( nanophemera ) OR TITLE-ABS-KEY ( nanophthalm\* ) OR

TITLE-ABS-KEY ( nanophya ) OR TITLE-ABS-KEY ( nanophydes ) OR TITLE-ABS-KEY ( nanophydinae )  
OR TITLE-ABS-KEY ( nanophydini ) OR TITLE-ABS-KEY ( nanophyes ) OR TITLE-ABS-KEY ( nanophyetinae ) OR TITLE-ABS-KEY ( nanophyetus ) OR TITLE-ABS-KEY ( nanophyidae ) OR TITLE-ABS-KEY ( nanophyinae ) OR TITLE-ABS-KEY ( nanophyini ) OR TITLE-ABS-KEY ( nanophylla ) OR TITLE-ABS-KEY ( nanophylliini ) OR TITLE-ABS-KEY ( nanophyllum ) OR TITLE-ABS-KEY ( nanophyllum ) OR TITLE-ABS-KEY ( nanophyllus ) OR TITLE-ABS-KEY ( nanophytes ) )

#8

(TITLE-ABS-KEY ( nanophyti ) OR TITLE-ABS-KEY ( nanophyto\* ) OR TITLE-ABS-KEY ( nanopilumnus ) OR TITLE-ABS-KEY ( nanopitar ) OR TITLE-ABS-KEY ( nanoplagia ) OR TITLE-ABS-KEY ( nanoplax ) OR TITLE-ABS-KEY ( nanoplaxes ) OR TITLE-ABS-KEY ( nanoplectrus ) OR TITLE-ABS-KEY ( nanoplithisus ) OR TITLE-ABS-KEY ( nanopodella ) OR TITLE-ABS-KEY ( nanopodellus ) OR TITLE-ABS-KEY ( nanopolymorphum ) OR TITLE-ABS-KEY ( nanopolystoma ) OR TITLE-ABS-KEY ( nanopria ) OR TITLE-ABS-KEY ( nanoprotist\* ) OR TITLE-ABS-KEY ( nanops ) OR TITLE-ABS-KEY ( nanopsallus ) OR TITLE-ABS-KEY ( nanopsis ) OR TITLE-ABS-KEY ( nanopsocetae ) OR TITLE-ABS-KEY ( nanopsocus ) OR TITLE-ABS-KEY ( nanopterodectes ) OR TITLE-ABS-KEY ( nanopterum ) OR TITLE-ABS-KEY ( nanoptilium ) OR TITLE-ABS-KEY ( nanopus ) OR TITLE-ABS-KEY ( nanopyxis ) OR TITLE-ABS-KEY ( nanoqia ) OR TITLE-ABS-KEY ( nanoqsunquak ) OR TITLE-ABS-KEY ( nanor ) OR TITLE-ABS-KEY ( nanorafonus ) OR TITLE-ABS-KEY ( nanorana ) OR TITLE-ABS-KEY ( nanoraphidia ) OR TITLE-ABS-KEY ( nanorchestes ) OR TITLE-ABS-KEY ( nanorchestidae ) OR TITLE-ABS-KEY ( nanorhamphus ) )

#9

(TITLE-ABS-KEY ( nanorhathymus ) OR TITLE-ABS-KEY ( nanorhopaea ) OR TITLE-ABS-KEY ( nanorrhacus ) OR TITLE-ABS-KEY ( nanorrhynchus ) OR TITLE-ABS-KEY( Nanorthidae ) OR TITLE-ABS-KEY( Nanorthis ) OR TITLE-ABS-KEY( Nanos ) OR TITLE-ABS-KEY( Nanosalicium ) OR TITLE-ABS-KEY( Nanosatellite\* ) OR TITLE-ABS-KEY( Nanosauridae ) OR TITLE-ABS-KEY( Nanosaurus ) OR TITLE-ABS-KEY( Nanoschema ) OR TITLE-ABS-KEY( Nanoschetus ) OR TITLE-ABS-KEY( Nanoscydmus ) OR TITLE-ABS-KEY( Nanoscypha ) OR TITLE-ABS-KEY("nano-second\*" ) OR TITLE-ABS-KEY( Nanosecond\* ) OR TITLE-ABS-KEY( Nanosella ) OR TITLE-ABS-KEY( Nanosellini ) OR TITLE-ABS-KEY( Nanoserranus ) OR TITLE-ABS-KEY( Nanosesarma ) OR TITLE-ABS-KEY( Nanosetus ) OR TITLE-ABS-KEY( Nanosilene ) OR TITLE-ABS-KEY("nano-SIMS" ) OR TITLE-ABS-KEY( Nanosiren ) OR TITLE-ABS-KEY( Nanosius ) OR TITLE-ABS-KEY( Nanosmia ) OR TITLE-ABS-KEY( Nanosmilus ) OR TITLE-ABS-KEY( Nanosomus ) OR TITLE-ABS-KEY( Nanospadix ) OR TITLE-ABS-KEY( Nanospathulatum ) OR TITLE-ABS-KEY( Nanospira ) OR TITLE-

ABS-KEY( Nanospondylus ) OR TITLE-ABS-KEY( Nanospora ) OR TITLE-ABS-KEY( Nanospray\* ) OR TITLE-ABS-KEY("nano-spray\*" ) OR TITLE-ABS-KEY( Nanosteatoda ) OR TITLE-ABS-KEY( Nanostellata ) OR TITLE-ABS-KEY( Nanostictis ))

#10

(TITLE-ABS-KEY( Nanostoma ) OR TITLE-ABS-KEY( Nanostomus ) OR TITLE-ABS-KEY( Nanostrangalia ) OR TITLE-ABS-KEY( Nanostrea ) OR TITLE-ABS-KEY( Nanostreptus ) OR TITLE-ABS-KEY( Nanosura ) OR TITLE-ABS-KEY( Nanosylvanella ) OR TITLE-ABS-KEY( Nanotagalus ) OR TITLE-ABS-KEY( Nanotanaupodus ) OR TITLE-ABS-KEY( Nanotaphus ) OR TITLE-ABS-KEY( Nanotermitodius ) OR TITLE-ABS-KEY( Nanothamnus ) OR TITLE-ABS-KEY( Nanothecioidea ) OR TITLE-ABS-KEY( Nanothecium ) OR TITLE-ABS-KEY( Nanothinophilus ) OR TITLE-ABS-KEY( Nanothrips ) OR TITLE-ABS-KEY( Nanothyris ) OR TITLE-ABS-KEY( Nanotitan ) OR TITLE-ABS-KEY( Nanotitanops ) OR TITLE-ABS-KEY( Nanotopsis ) OR TITLE-ABS-KEY( Nanotragulus ) OR TITLE-ABS-KEY( Nanotragus ) OR TITLE-ABS-KEY( Nanotrema ) OR TITLE-ABS-KEY( Nanotrepes ) OR TITLE-ABS-KEY( Nanotrigona ) OR TITLE-ABS-KEY( Nanotriton ) OR TITLE-ABS-KEY( Nanotrombium ) OR TITLE-ABS-KEY( Nanotyranus ) OR TITLE-ABS-KEY( Nanoviridae ) OR TITLE-ABS-KEY( Nanovirus ) OR TITLE-ABS-KEY( Nanowana ) OR TITLE-ABS-KEY( Nanowestratia ) OR TITLE-ABS-KEY( Nanoxylocopa ) OR TITLE-ABS-KEY( Nano2 ) OR TITLE-ABS-KEY( Nano3 ) OR TITLE-ABS-KEY(plankton\* ) OR TITLE-ABS-KEY( "N\*plankton\*" ) OR TITLE-ABS-KEY("m\*plankton\*" ) OR TITLE-ABS-KEY("b\*plankton\*" ) OR TITLE-ABS-KEY("p\*plankton\*" ) OR TITLE-ABS-KEY("z\*plankton\*" ))

#11= #1 AND NOT (#2 OR #3 OR #4 OR #5 OR #6 OR #7 OR #8 OR #9 OR #10)

#12

(( (TITLE-ABS-KEY( gadonano\* ) OR TITLE-ABS-KEY( glyconanopartic\* ) OR TITLE-ABS-KEY( heteronano\* ) OR TITLE-ABS-KEY( immunonanogold ) OR TITLE-ABS-KEY( immunonanopartic\* ) OR TITLE-ABS-KEY( polynanocrystal\* ) OR TITLE-ABS-KEY( subnanocluster\* ) OR TITLE-ABS-KEY( ultrananocrystal\* ) OR TITLE-ABS-KEY( ultrananodiamond\* )) ) OR (( (TITLE-ABS-KEY( "self assembl\*" ) OR TITLE-ABS-KEY( "self organiz\*" ) OR TITLE-ABS-KEY( "directed assembl\*" )) ) AND ( (TITLE-ABS-KEY( monolayer\* ) OR TITLE-ABS-KEY( "mono-layer\*" ) OR TITLE-ABS-KEY( film\* ) OR TITLE-ABS-KEY( quantum\* ) OR TITLE-ABS-KEY( multilayer\* ) OR TITLE-ABS-KEY( "multi-layer\*" ) OR TITLE-ABS-KEY( array ) OR TITLE-ABS-KEY( molecu\* ) OR TITLE-ABS-KEY( polymer\* ) OR TITLE-ABS-KEY( "co-polymer\*" ) OR TITLE-ABS-KEY( copolymer\* ) OR TITLE-ABS-KEY( mater\* ) OR TITLE-ABS-KEY( biolog\* ) OR TITLE-ABS-KEY( supramolecul\* )) )) ) AND NOT ( TITLE-ABS-KEY( nano\* ) )

#13

( ( TITLE-ABS-KEY ( "quantum dot\*" ) OR TITLE-ABS-KEY ( "quantum well\*" ) OR TITLE-ABS-KEY ( "quantum wire\*" ) OR TITLE-ABS-KEY ( "molecul\* motor\*" ) OR TITLE-ABS-KEY ( "molecul\* ruler\*" ) OR TITLE-ABS-KEY ( "molecul\* wir\*" ) OR TITLE-ABS-KEY ( "molecul\* devic\*" ) OR TITLE-ABS-KEY ( "molecular engineering" ) OR TITLE-ABS-KEY ( "molecular electronic\*" ) OR TITLE-ABS-KEY ( "single molecul\*" ) OR TITLE-ABS-KEY ( fulleren\* ) OR TITLE-ABS-KEY ( buckyball ) OR TITLE-ABS-KEY ( buckminsterfullerene ) OR TITLE-ABS-KEY ( "C-60" ) OR TITLE-ABS-KEY ( c70 ) OR TITLE-ABS-KEY ( c120 ) OR TITLE-ABS-KEY ( swcnt ) OR TITLE-ABS-KEY ( mwcnt ) OR TITLE-ABS-KEY ( "coulomb blockad\*" ) OR TITLE-ABS-KEY ( bionano\* ) OR TITLE-ABS-KEY ( "Langmuir-blodgett" ) OR TITLE-ABS-KEY ( coulombstaircase\* ) OR TITLE-ABS-KEY ( "coulomb-staircase" ) OR TITLE-ABS-KEY ( "PDMS stamp\*" ) OR TITLE-ABS-KEY ( graphene ) OR TITLE-ABS-KEY ( "dye-sensitized solar cell" ) OR TITLE-ABS-KEY ( dssc ) OR TITLE-ABS-KEY ( ferrofluid\* ) OR TITLE-ABS-KEY ( fullerid\* ) OR TITLE-ABS-KEY ( fullerinol\* ) OR TITLE-ABS-KEY ( fullerite\* ) OR TITLE-ABS-KEY ( fullerol\* ) OR TITLE-ABS-KEY ( fulleropyrrolidin\* ) OR TITLE-ABS-KEY ( "core-shell" ) OR TITLE-ABS-KEY ( nems ) OR TITLE-ABS-KEY ( "atom\* scale" ) OR TITLE-ABS-KEY ( "ballistic transport\*" ) OR TITLE-ABS-KEY ( "DNA comput\*" ) OR TITLE-ABS-KEY ( "porous silicon" ) OR TITLE-ABS-KEY ( "a\*fulleren\*" ) OR TITLE-ABS-KEY ( "b\*fulleren\*" ) OR TITLE-ABS-KEY ( "c\*fulleren\*" ) OR TITLE-ABS-KEY ( "d\*fulleren\*" ) OR TITLE-ABS-KEY ( "e\*fulleren\*" ) OR TITLE-ABS-KEY ( "f\*fulleren\*" ) OR TITLE-ABS-KEY ( "g\*fulleren\*" ) OR TITLE-ABS-KEY ( "h\*fulleren\*" ) OR TITLE-ABS-KEY ( "i\*fulleren\*" ) OR TITLE-ABS-KEY ( "j\*fulleren\*" ) OR TITLE-ABS-KEY ( "k\*fulleren\*" ) OR TITLE-ABS-KEY ( "l\*fulleren\*" ) OR TITLE-ABS-KEY ( "m\*fulleren\*" ) OR TITLE-ABS-KEY ( "n\*fulleren\*" ) OR TITLE-ABS-KEY ( "o\*fulleren\*" ) OR TITLE-ABS-KEY ( "p\*fulleren\*" ) OR TITLE-ABS-KEY ( "q\*fulleren\*" ) OR TITLE-ABS-KEY ( "r\*fulleren\*" ) OR TITLE-ABS-KEY ( "s\*fulleren\*" ) OR TITLE-ABS-KEY ( "t\*fulleren\*" ) OR TITLE-ABS-KEY ( "u\*fulleren\*" ) OR TITLE-ABS-KEY ( "v\*fulleren\*" ) OR TITLE-ABS-KEY ( "w\*fulleren\*" ) OR TITLE-ABS-KEY ( "x\*fulleren\*" ) OR TITLE-ABS-KEY ( "y\*fulleren\*" ) OR TITLE-ABS-KEY ( "z\*fulleren\*" ) ) OR ( ( TITLE-ABS-KEY ( c60 ) ) AND NOT ( TITLE-ABS-KEY ( c60 ) AND TITLE-ABS-KEY ( steel ) ) ) ) AND NOT ( TITLE-ABS-KEY ( nano\* ) )

#14

( ( TITLE-ABS-KEY ( tem ) OR TITLE-ABS-KEY ( stm ) OR TITLE-ABS-KEY ( edx ) OR TITLE-ABS-KEY ( afm ) OR TITLE-ABS-KEY ( hrtem ) OR TITLE-ABS-KEY ( sem ) OR TITLE-ABS-KEY ( eels ) OR TITLE-ABS-KEY ( sers ) OR TITLE-ABS-KEY ( mfm ) OR TITLE-ABS-KEY ( uv-vis ) OR TITLE-ABS-KEY ( xps ) OR TITLE-ABS-KEY ( nsom ) OR TITLE-ABS-KEY ( "atom\* force microscop\*" ) OR TITLE-ABS-KEY ( "tunnel\* microscop\*" ) OR TITLE-ABS-KEY ( "scanning probe microscop\*" ) OR TITLE-ABS-KEY ( "transmission



electron microscop\*" ) OR TITLE-ABS-KEY ( "scanning electron microscop\*" ) OR TITLE-ABS-KEY ( "energy dispersive X-ray" ) OR TITLE-ABS-KEY ( "xray photoelectron\*" ) OR TITLE-ABS-KEY ( "x-ray photoelectron" ) OR TITLE-ABS-KEY ( "electron energy loss spectroscop\*" ) OR TITLE-ABS-KEY ( "enhanced raman-scattering" ) OR TITLE-ABS-KEY ( "surface enhanced raman scattering" ) OR TITLE-ABS-KEY ( "single molecule microscopy" ) OR TITLE-ABS-KEY ( "focused ion beam" ) OR TITLE-ABS-KEY ( "ellipsometry" ) OR TITLE-ABS-KEY ( "magnetic force microscopy" ) OR TITLE-ABS-KEY ( "UV-Visible Spectroscop\*" ) OR TITLE-ABS-KEY ( "Ultraviolet-visible spectroscop\*" ) OR TITLE-ABS-KEY ( "near field scanning optical microscop\*" ) OR TITLE-ABS-KEY ( pebbles ) OR TITLE-ABS-KEY ( quasicrystal\* ) OR TITLE-ABS-KEY ( "quasi-crystal\*" ) ) AND ( TITLE-ABS-KEY ( monolayer\* ) OR TITLE-ABS-KEY ( "mono-layer\*" ) OR TITLE-ABS-KEY ( film\* ) OR TITLE-ABS-KEY ( quantum\* ) OR TITLE-ABS-KEY ( multilayer\* ) OR TITLE-ABS-KEY ( "multi-layer\*" ) OR TITLE-ABS-KEY ( array\* ) ) AND NOT ( TITLE-ABS-KEY ( nano\* ) )

#15

(( TITLE-ABS-KEY ( biosensor\* ) OR TITLE-ABS-KEY ( nems ) OR TITLE-ABS-KEY ( "sol gel\*" ) OR TITLE-ABS-KEY ( "solgel\*" ) OR TITLE-ABS-KEY ( dendrimer\* ) OR TITLE-ABS-KEY ( "soft lithograph\*" ) OR TITLE-ABS-KEY ( "molecular simul\*" ) OR TITLE-ABS-KEY ( "molecular machin\*" ) OR TITLE-ABS-KEY ( "molecular imprinting" ) OR TITLE-ABS-KEY ( "quantum effect\*" ) OR TITLE-ABS-KEY ( "molecular sieve\*" ) OR TITLE-ABS-KEY ( "surface energy" ) OR TITLE-ABS-KEY ( "mesoporous material\*" ) OR TITLE-ABS-KEY ( "mesoporous silica" ) OR TITLE-ABS-KEY ( "porous silicon" ) OR TITLE-ABS-KEY ( "zeta potential" ) OR TITLE-ABS-KEY ( "epitax\*" ) OR TITLE-ABS-KEY ( cnt ) OR TITLE-ABS-KEY ( "electron beam lithography" ) OR TITLE-ABS-KEY ( "e-beam lithography" ) OR TITLE-ABS-KEY ( "quantum size effect" ) OR TITLE-ABS-KEY ( "quantum device" ) OR TITLE-ABS-KEY ( "chemical vapor deposition" ) OR TITLE-ABS-KEY ( cvd ) OR TITLE-ABS-KEY ( "chemical vapour deposition" ) OR TITLE-ABS-KEY ( "surface plasmon resonance" ) OR TITLE-ABS-KEY ( "differential scanning calorimetry" ) ) AND ( TITLE-ABS-KEY ( monolayer\* ) OR TITLE-ABS-KEY ( "mono-layer\*" ) OR TITLE-ABS-KEY ( film\* ) OR TITLE-ABS-KEY ( quantum\* ) OR TITLE-ABS-KEY ( multilayer\* ) OR TITLE-ABS-KEY ( "multi-layer\*" ) OR TITLE-ABS-KEY ( array\* ) ) AND NOT ( TITLE-ABS-KEY ( nano\* ) )

FINAL QUERY (#11 OR #12 OR #13 OR #14 OR #15)

## Lexical queries for WOS

#1

TS=nano\*

#2

TS=((gadonano\* OR glyconanopartic\* OR heteronano\* OR immunonanogold OR immunonopartic\*) OR ("self assembl\*" OR "self organiz\*" OR "directed assembl\*") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array OR molecu\* OR polymer\* OR "co-polymer\*" OR copolymer\* OR mater\* OR biolog\* OR supramolecul\*))

#3

TS=(( polynanocrystal\* OR subnanocluster\* OR ultrananocrystal\* OR ultrananodiamond\*) OR ("self assembl\*" OR "self organiz\*" OR "directed assembl\*") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array OR molecu\* OR polymer\* OR "co-polymer\*" OR copolymer\* OR mater\* OR biolog\* OR supramolecul\*))

#4

TS=("quantum dot\*" OR "quantum well\*" OR "quantum wire\*" OR "molecul\* motor\*" OR "molecul\* ruler\*" OR "molecul\* wir\*" OR "molecul\* devic\*" OR "molecular engineering" OR "molecular electronic\*" OR "single molecul\*")

#5

TS=(fulleren\* OR buckyball OR buckminsterfullerene OR "C-60" OR (c60 NOT(c60 AND steel)) OR c70 OR c120 OR swcnt OR mwcnt)

#6

TS=("coulomb blockad\*" OR bionano\* OR "Langmuir-blodgett" OR coulombstaircase\* OR "coulomb-staircase" OR "PDMS stamp\*" OR graphene OR "dye-sensitized solar cell" OR dssc OR ferrofluid\*)

#7

TS=(fullerid\* OR fullerinol\* OR fullerite\* OR fullerol\* OR fulleropyrrolidin\* OR "core-shell" OR nems OR "atom\* scale" OR "ballistic transport\*" OR "DNA comput\*")

#8

TS=("porous silicon" OR "a\*fulleren\*" OR "b\*fulleren\*" OR "c\*fulleren\*" OR "d\*fulleren\*" OR "e\*fulleren\*" OR "f\*fulleren\*" OR "g\*fulleren\*" OR "h\*fulleren\*" OR "i\*fulleren\*")

#9

TS=("j\*fulleren\*" OR "k\*fulleren\*" OR "l\*fulleren\*" OR "m\*fulleren\*" OR "n\*fulleren\*" OR "o\*fulleren\*" OR "p\*fulleren\*" OR "q\*fulleren\*" OR "r\*fulleren\*" OR "s\*fulleren\*")

#10

TS=("t\*fulleren\*" OR "u\*fulleren\*" OR "v\*fulleren\*" OR "w\*fulleren\*" OR "x\*fulleren\*" OR "y\*fulleren\*" OR "z\*fulleren\*")

#11

TS=((tem OR stm OR edx OR afm OR hrtem OR sem) AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#12

TS=((eels OR sers OR mfm OR uv-vis OR xps OR nsom) AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#13

TS(("atom\* force microscop\*" OR "tunnel\* microscop\*" OR "scanning probe microscop\*" OR "transmission electron microscop\*" OR "scanning electron microscop\*") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#14

TS(("energy dispersive X-ray" OR "xray photoelectron\*" OR "x-ray photoelectron" OR "electron energy loss spectroscop\*") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#15

TS=("enhanced raman-scattering" OR "surface enhanced raman scattering" OR "single molecule microscopy" OR "focused ion beam") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#16

TS=("ellipsometry" OR "magnetic force microscopy" OR "UV-Visible Spectroscop\*") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#17

TS=("Ultraviolet-visible spectroscop\*" OR "near field scanning optical microscop\*" OR pebbles OR quasicrystal\* OR "quasi-crystal\*") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#18

TS=((biosensor\* OR nems OR "sol gel\*" OR "solgel\*" OR dendrimer\*) AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#19

TS=("soft lithograph\*" OR "molecular simul\*" OR "molecular machin\*" OR "molecular imprinting" OR "quantum effect\*") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#20

TS=("molecular sieve\*" OR "surface energy" OR "mesoporous material\*" OR "mesoporous silica" OR "porous silicon") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#21

TS=("zeta potential" OR "epitax\*" OR cnt OR "electron beam lithography" OR "e-beam lithography") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#22

TS=(("quantum size effect" OR "quantum device" OR "chemical vapor deposition" OR cvd OR "chemical vapour deposition" OR "surface plasmon resonance" OR "differential scanning calorimetry") AND (monolayer\* OR "mono-layer\*" OR film\* OR quantum\* OR multilayer\* OR "multi-layer\*" OR array\*))

#23

TS=(nanao OR nanoacalles OR nanoagraylea OR nanoalga\* OR nanoapiculatum OR nanoarchaeaor OR nanoarchaeota OR nanoarchaeum OR nanoastegotherium OR "nano\*aryote\*")

#24

TS=(nanobacteri\* OR nanobagrus OR nanobalcis OR nanobaris OR nanobates OR nanobatinae OR nanobius OR nanobryaceae OR nanobryoides OR nanobuthus)

#25

TS=(nano-bible OR nanocalcar OR nanocambridgea OR nanocapillare OR nanocapillary OR nanocarpa OR nanocarpum OR nanocarpus OR nanocassiope OR nanocavia OR nanocephalum OR nanocheiroduon)

#26

TS=(nanochilina OR nanochilus OR nanochitina OR nanochlaenius OR nanochlorum OR nanochoerus OR nanochromis OR nanochromosom\* OR nanochrysopa OR nanochthonius)

#27

TS=(nanocixius OR nanocladius OR nanoclarella OR nanoclavelia OR nanoclimacium OR nanoclymenia OR nanocnide OR nanocochlea OR nanocolletes OR nanocondylodesmus)

#28

TS=(nanocopia OR nanocoquimba OR nanocrinus OR nanoctenus OR nanocthispa OR nanocuridae OR nanocurie OR nano-curie OR nanocuris OR nanocyclopia OR nanocynodon OR nanocythere)

#29

TS=(nanodacna OR nanodactylus OR nanodamon OR nanodea OR nanodealbata OR nanodectes OR nanodella OR nanodelphys OR nanodendron OR nanodes)

#30

TS=(nanodiaparsis OR nanodiaptomus OR nanodidelphys OR nanodiella OR nanodiodes OR nanodiplois OR nanodiscus OR nanodisticha OR nanodromia OR nanodynerus)

#31

TS=(nanoesi OR nanofauna\* OR nanofila OR "nano-filt\*" OR nanofilt\* OR nanoflagel\* OR nanoflow OR "nano-flow" OR nanofilidae OR Nanog OR Nanog1)

#32

TS=(Nanog2 OR Nanogalatea OR Nanogeterotroph\* OR Nanoglobum OR Nanoglossa OR Nanognathia OR Nanognathus OR Nanogomphodon OR Nanogona OR Nanogonalos)

#33

TS=(Nanogorgon OR Nanogram\* OR "nano-gram\*" OR Nanogramma OR Nanograptus OR Nanogyra OR Nanogryrini OR Nanohalus OR Nanohammus OR Nanohemicera)

#34

TS=(Nanoheterotroph\* OR Nanohystrix OR Nanoides OR Nanoini OR Nanojapyx OR Nanokerala OR Nanokelvin\* OR Nanokermes OR Nanola OR Nanolachesilla)

#35

TS=(Nanolania OR Nanolauthia OR NanoLC\* OR "nano-LC\*" OR Nanolestes OR Nanolichus OR "nanoliter\*" OR "nano-litre\*" OR Nanoliter\* OR Nanolitre\* OR Nanolobus OR Nanoloricida)

#36

TS=(Nanolpium OR Nanolumen OR Nanomaja OR Nanomantinae OR Nanomantini OR Nanomantis OR Nanomeli\* OR Nanomelon OR Nanomermis OR Nanomerus OR Nanomeryx OR Nanometa)

#37

TS=("nano-meter\*" OR Nanometidae OR Nanometinae OR Nanometra OR "nano-metre\*" OR "nm"  
OR Nanometer\* OR Nanometre\* OR Nanomia OR Nanomias OR Nanomicrophytes)

#38

TS=(Nanomilleretta OR Nanomimus OR Nanomis OR Nanomitra OR Nanomitriella OR Nanomitriopsis  
OR Nanomitus OR Nanomol\* OR "nano-molar" OR "nano-mole\*")

#39

TS=(Nanomutilinae OR Nanomutilla OR Nanomyces OR Nanomyina OR Nanomyrmacyba OR  
Nanomyrme OR Nanomys OR Nanomysis OR Nanomysmena)

#40

TS=(Nanonaucoris OR Nanonavis OR Nanoneis OR Nanonemoura OR Nanonocticolus OR Nanonycteris  
OR "Nanook of the North" OR nanopachyiulus OR nanopagurus OR nanopareia)

#41

TS=(nanoparia OR nanopatula OR nanopennatum OR nanoperla OR nanophareus OR nanophemera  
OR nanophtalm\* OR nanophya OR nanophydes OR nanophydinae)

#42

TS=(nanophydini OR nanophyes OR nanophyetinae OR nanophyetus OR nanophyidae OR  
nanophyinae OR nanophyini OR nanophylla OR nanophylliini OR nanophyllum OR nanophyllum OR  
nanophyllus OR nanophytes)

#43

TS=(nanophyti OR nanophyto\* OR nanopilumnus OR nanopitar OR nanoplagia OR nanoplax OR  
nanoplaxes OR nanoplectrus OR nanoplinthisus OR nanopodella OR nanopodellus OR  
nanopolymorphum)

#44

TS=(nanopolystoma OR nanopria OR nanoprotist\* OR nanops OR nanopsallus OR nanopsis OR nanopsocetae OR nanopsocus OR nanopterodectes OR nanopterum)

#45

TS=(nanoptilium OR nanopus OR nanopyxis OR nanoqia OR nanoqsunquak OR nanor OR nanorafonus OR nanorana OR nanoraphidia OR nanorchestes OR nanorchestidae OR nanorhamphus)

#46

TS=(nanorhathymus OR nanorhopaea OR nanorrhacus OR nanorrhynchus OR Nanorthidae OR Nanorthis OR Nanos OR Nanosalicium OR Nanosatellite\* OR Nanosauridae OR Nanosaurus)

#47

TS=(Nanoschema OR Nanoschetus OR Nanoscydmus OR Nanoscypha OR "nano-second\*" OR Nanosecond\* OR Nanosella OR Nanosellini OR Nanoserranus OR Nanosesarma OR Nanosetus)

#48

TS=(Nanosilene OR "nano-SIMS" OR Nanosiren OR Nanosius OR Nanosmia OR Nanosmilus OR Nanosomus OR Nanospadix OR Nanospathulatum OR Nanospira)

#49

TS=(Nanospondylus OR Nanospora OR Nanospray\* OR "nano-spray\*" OR Nanosteatoda OR Nanostellata OR Nanostictis)

#50

TS=(Nanostoma OR Nanostomus OR Nanostrangalia OR Nanostrea OR Nanostreptus OR Nanosura OR Nanosylvanella OR Nanotagalus OR Nanotanaupodus OR Nanotaphus)

#51

TS=(Nanotermitodius OR Nanothamnus OR Nanothecioidea OR Nanothecium OR Nanothinophilus OR Nanothrips OR Nanothyris OR Nanotitan OR Nanotitanops)

#52



TS=(Nanotopsis OR Nanotragulus OR Nanotragus OR Nanotrema OR Nanotrepes OR Nanotrigona OR Nanotriron OR Nanotrombium OR Nanotyrannus OR Nanoviridae)

#53

TS=(Nanovirus OR Nanowana OR Nanowestratia OR Nanoxylocopa OR Nano2 OR Nano3 OR plankton\* OR "N\*plankton\*" OR "m\*plankton\*" OR "b\*plankton\*" OR "p\*plankton\*" OR "z\*plankton\*")

FINAL QUERY (#1 OR #2 OR #3 OR #4 OR #5 OR #6 OR #7 OR #8 OR #9 OR #10 OR #11 OR #12 OR #13 OR #14 OR #15 OR #16 OR #17 OR #18 OR #19 OR #21 OR #22) NOT (#23 OR #24 OR #25 OR #26 OR #27 OR #28 OR #29 OR #30 OR #31 OR #32 OR #33 OR #34 OR #35 OR #36 OR #37 OR #38 OR #39 OR #40 OR #41 OR #42 OR #43 OR #44 OR #45 OR #46 OR #47 OR #48 OR #49 OR #50 OR #51 OR #52 OR #53)

### **Appendix 3. Journals list with nano prefix in their titles retrieved from WoS and Scopus**

<i>Journals list with nano prefix in their titles</i>
ACS NANO*
ADVANCES IN NATURAL SCIENCES NANOSCIENCE AND NANOTECHNOLOGY
APPLIED NANOSCIENCE
ARTIFICIAL CELLS NANOMEDICINE AND BIOTECHNOLOGY
BEILSTEIN JOURNAL OF NANOTECHNOLOGY
BIOINSPIRED BIOMIMETIC AND NANOBIMATERIALS
CANCER NANOTECHNOLOGY
CHEMNANOMAT
CURRENT NANOSCIENCE
DIGEST JOURNAL OF NANOMATERIALS AND BIOSTRUCTURES
E JOURNAL OF SURFACE SCIENCE AND NANOTECHNOLOGY
ENVIRONMENTAL NANOTECHNOLOGY MONITORING AND MANAGEMENT
ENVIRONMENTAL SCIENCE NANO
FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES
IEEE NANOTECHNOLOGY MAGAZINE
IEEE TRANSACTIONS ON NANOBIOSCIENCE
IEEE TRANSACTIONS ON NANOTECHNOLOGY
IET NANOBIOENGINEERING
INORGANIC AND NANO METAL CHEMISTRY
INTEGRATIVE BIOLOGY – QUANTITATIVE BIOSCIENCE FROM NANO TO MACRO
INTERNATIONAL JOURNAL OF BIOMEDICAL NANOSCIENCE AND NANOTECHNOLOGY
INTERNATIONAL JOURNAL OF NANO AND BIOMATERIALS
INTERNATIONAL JOURNAL OF NANOELECTRONICS AND MATERIALS

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*Journals list with nano prefix in their titles*

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INTERNATIONAL JOURNAL OF NANOMANUFACTURING  
INTERNATIONAL JOURNAL OF NANOMEDICINE  
INTERNATIONAL JOURNAL OF NANOPARTICLES  
INTERNATIONAL JOURNAL OF NANOSCIENCE  
INTERNATIONAL JOURNAL OF NANOTECHNOLOGY  
INTERNATIONAL JOURNAL OF SMART AND NANO MATERIALS  
JOURNAL OF BIOMEDICAL NANOTECHNOLOGY  
JOURNAL OF BIONANOSCIENCE  
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE  
JOURNAL OF EXPERIMENTAL NANOSCIENCE  
JOURNAL OF LASER MICRO NANOENGINEERING  
JOURNAL OF MICRO NANOLITHOGRAPHY MEMS AND MOEMS  
JOURNAL OF MICRO-BIO ROBOTICS  
JOURNAL OF NANO AND ELECTRONIC PHYSICS  
JOURNAL OF NANO RESEARCH  
JOURNAL OF NANOBIO TECHNOLOGY  
JOURNAL OF NANO ELECTRONICS AND OPTOELECTRONICS  
JOURNAL OF NANOMATERIALS  
JOURNAL OF NANOMECHANICS AND MICROMECHANICS  
JOURNAL OF NANOMEDICINE AND NANOTECHNOLOGY  
JOURNAL OF NANOPARTICLE RESEARCH  
JOURNAL OF NANOPHOTONICS  
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY  
JOURNAL OF NANOTECHNOLOGY  
JOURNAL OF VACUUM SCIENCE AND TECHNOLOGY B NANOTECHNOLOGY AND MICROELECTRONICS  
MICRO AND NANO LETTERS  
MICRO AND NANOSYSTEMS  
MICROFLUIDICS AND NANOFUIDICS  
MICROSYSTEM TECHNOLOGIES-MICRO-AND NANOSYSTEMS-INFORMATION STORAGE AND  
PROCESSING SYSTEMS  
NAMI JISHU YU JINGMI GONGCHENG NANOTECHNOLOGY AND PRECISION ENGINEERING  
NANO  
NANO BIOMEDICINE  
NANO BIOMEDICINE AND ENGINEERING  
NANO COMMUNICATION NETWORKS  
NANO ENERGY  
NANO LETTER\* °  
NANO LIFE  
NANO MICRO LETTERS  
NANO RESEARCH  
NANO STRUCTURES AND NANO OBJECTS  
NANO TODAY

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*Journals list with nano prefix in their titles*

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**NANOETHICS**

**NANOIMPACT**

**NANOMATERIALS**

**NANOMATERIALS AND NANOTECHNOLOGY**

**NANOMEDICINE**

**NANOMEDICINE NANOTECHNOLOGY BIOLOGY AND MEDICINE**

**NANOPHOTONICS**

**NANOSCALE AND MICROSCALE THERMOPHYSICAL ENGINEERING**

**NANOSCALE RESEARCH LETTERS**

**NANOSCALE\***

**NANOSCIENCE AND NANOTECHNOLOGY ASIA**

**NANOSCIENCE AND NANOTECHNOLOGY LETTERS**

**NANOSCIENCE AND TECHNOLOGY: AN INTERNATIONAL JOURNAL (INTERNATIONAL JOURNAL OF NANOMECHANICS SCIENCE AND TECHNOLOGY**

**NANOTECHNOLOGIES IN RUSSIA**

**NANOTECHNOLOGY**

**NANOTECHNOLOGY PERCEPTIONS**

**NANOTECHNOLOGY REVIEWS**

**NANOTECHNOLOGY SCIENCE AND APPLICATIONS**

**NANOTOXICOLOGY**

**NATURE NANOTECHNOLOGY**

**OPENNANO**

**PHOTONICS AND NANOSTRUCTURES FUNDAMENTALS AND APPLICATIONS**

**PHYSICA E LOW DIMENSIONAL SYSTEMS AND NANOSTRUCTURES**

**PRECISION ENGINEERING-JOURNAL OF THE INTERNATIONAL SOCIETIES FOR PRECISION ENGINEERING AND NANOTECHNOLOGY**

**PROCEEDINGS OF THE INSTITUTION OF MECHANICAL ENGINEERS, PART N: JOURNAL OF NANOMATERIALS, NANOENGINEERING AND NANOSYSTEMS**

**RECENT PATENTS ON NANOTECHNOLOGY**

**WILEY INTERDISCIPLINARY REVIEWS NANOMEDICINE AND NANOBIOTECHNOLOGY**

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<sup>o</sup> Identified by elbow criterion with threshold kink from NST WoS data set

\*Identified by elbow criterion with threshold from NST Scopus data set

**Appendix 4. Identified journals by the elbow criterion with threshold kink by figures**

FIGURE 2	p	FIGURE 4	p	FIGURE 3	p	FIGURE 5	p
ACS APPLIED MATERIALS AND INTERFACES	1	ACS NANO	1	ADVANCED MATERIALS	1	APPLIED PHYSICS LETTERS	0.5
ACS NANO	1	ACTA MATERIALIA	0.5	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	0	ACS NANO	1
ADVANCED MATERIALS	1	ADVANCED MATERIALS	0.5	APPLIED PHYSICS LETTERS	0.5	ADVANCED MATERIALS	1
ANGEWANDTE CHEMIE - INTERNATIONAL EDITION	0	ANALYTICAL CHEMISTRY	0	CHEMICAL COMMUNICATIONS	0	ANALYTICAL CHEMISTRY	0
APPLIED PHYSICS LETTERS	0.5	APPLIED PHYSICS LETTERS	0.5	CHEMISTRY OF MATERIALS	0	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	0
CHEMICAL COMMUNICATIONS	0	BIOMATERIALS	1	JOURNAL OF APPLIED PHYSICS	0.5	BIOMATERIALS	1
CHEMICAL SOCIETY REVIEWS	0	CHEMICAL COMMUNICATIONS	0	JOURNAL OF MATERIALS CHEMISTRY	0.5	CHEMICAL COMMUNICATIONS	0
JOURNAL OF PHYSICAL CHEMISTRY C	1	CHEMISTRY OF MATERIALS	0	JOURNAL OF PHYSICAL CHEMISTRY B	0	CHEMISTRY OF MATERIALS	0
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	0	JOURNAL OF APPLIED PHYSICS	0.5	JOURNAL OF PHYSICAL CHEMISTRY C	1	JOURNAL OF APPLIED PHYSICS	0.5
LANGMUIR	0.5	JOURNAL OF PHYSICAL CHEMISTRY B	0	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	0	JOURNAL OF PHYSICAL CHEMISTRY B	0
NANO LETTERS	1	JOURNAL OF PHYSICAL CHEMISTRY C	1	LANGMUIR	0.5	JOURNAL OF PHYSICAL CHEMISTRY C	1
NANOSCALE	1	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	0	MACROMOLECULES	0.5	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	0
PHYSICAL REVIEW B - CONDENSED MATTER AND MATERIALS PHYSICS	0.5	LANGMUIR	0.5	NANO LETTERS	1	LANGMUIR	0.5
		NANO LETTERS	1	PHYSICAL REVIEW B - CONDENSED MATTER AND MATERIALS PHYSICS	0.5	MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING	1
		NANOTECHNOLOGY	1	PHYSICAL REVIEW LETTERS	0	NANO LETTERS	1
		PHYSICAL REVIEW B - CONDENSED MATTER AND MATERIALS	0.5			PHYSICAL REVIEW B - CONDENSED MATTER AND MATERIALS	0.5

		PHYSICS				PHYSICS	
		PHYSICAL REVIEW LETTERS	0			PHYSICAL REVIEW LETTERS	0

### Appendix 5. Excluded journal from Step 5 to Step 7

Title journal	Excluded in Scopus data set	Excluded in WoS data set
ACM JOURNAL ON EMERGING TECHNOLOGIES IN COMPUTING SYSTEMS	x	x
ACS APPLIED MATERIALS & INTERFACES		x
ACS ENERGY LETTERS	x	x
ACS PHOTONICS	x	x
ACS SENSORS	x	x
ADVANCED ELECTRONIC MATERIALS	x	x
ADVANCED FUNCTIONAL MATERIALS	x	x
ADVANCED HEALTHCARE MATERIALS	x	x
ADVANCED SCIENCE	x	x
AIP ADVANCES	x	x
APL MATERIALS	x	x
BIOMEDICAL MICRODEVICES	x	x
BIOMICROFLUIDICS	x	x
BIOSENSORS & BIOELECTRONICS	x	x
JOURNAL OF BIOMEDICAL NANOTECHNOLOGY	x	
JOURNAL OF MICROELECTROMECHANICAL SYSTEMS	x	x
JOURNAL OF MICROMECHANICS AND MICROENGINEERING	x	x
JOURNAL OF NANO AND ELECTRONIC PHYSICS	x	
JOURNAL OF NANO RESEARCH	x	
JOURNAL OF PHYSICAL CHEMISTRY LETTERS	x	x
JOURNAL OF SURFACE INVESTIGATION	x	x
LAB ON A CHIP	x	x
MATERIALS EXPRESS	x	x
MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING	x	
MICROELECTRONIC ENGINEERING	x	x
MICROELECTRONICS JOURNAL	x	x
MICROELECTRONICS RELIABILITY	x	x
MICROMACHINES	x	x
MICROPOROUS AND MESOPOROUS MATERIALS	x	x
PARTICLE & PARTICLE SYSTEMS CHARACTERIZATION	x	x
PLASMONICS	x	x
REVIEWS ON ADVANCED MATERIALS SCIENCE	x	x
SCIENCE OF ADVANCED MATERIALS	x	x
SCRIPTA MATERIALIA	x	x
SMALL	x	x

## Appendix 6. Matching journals between all intersections

Title	ISSN	Thematic area	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	Scopus	Wos	Precision
ACS APPLIED MATERIALS & INTERFACES	1944-8244	Materials science (Nanomaterials)	x	x	x	Y	Y	1
ACS NANO	1936-0851	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
ACS PHOTONICS	2330-4022	Nanophotonics	x	x		Y	Y	1
ADVANCED MATERIALS	0935-9648	Materials science (Nanomaterials)	x	x	x	Y	Y	1
ADVANCED SCIENCE	2198-3844	Interdisciplinary (Materials science / Physics / Chemistry / Medicine / Engineering / Life Science)	x	x		Y	Y	1
ADVANCES IN NATURAL SCIENCES-NANOSCIENCE AND NANOTECHNOLOGY	2043-6262	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
APPLIED NANOSCIENCE	2190-5509	Nanoscience & Nanotechnology	x	x	x	N	Y	1
BEILSTEIN JOURNAL OF NANOTECHNOLOGY	2190-4286	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
CHEMNANOMAT	2199-692X	Materials science (Nanomaterials)	x	x	x	N	Y	1
CURRENT NANOSCIENCE	1573-4137	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
DIGEST JOURNAL OF NANOMATERIALS AND BIOSTRUCTURES	1842-3582	Nanomaterials	x		x	Y	Y	1
ENVIRONMENTAL SCIENCE-NANO	2051-8153	Nanoenvironment	x	x	x	Y	Y	1
FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES	1536-383X	Carbon materials	x	x	x	Y	Y	1
IEEE TRANSACTIONS ON NANOBIOSCIENCE	1536-1241	Nanomedicine	x	x	x	Y	Y	1
IEEE TRANSACTIONS ON NANOTECHNOLOGY	1536-125X	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
IET NANOBIOENGINEERING	1751-8741	Nanobiotechnology	x		x	Y	Y	1
INORGANIC AND NANO-METAL CHEMISTRY	1553-3174	Nanochemistry (Inorganic & nuclear chemistry)	x		x	Y	Y	1
INTERNATIONAL JOURNAL OF NANOMEDICINE	1176-9114	Nanomedicine	x		x	Y	Y	1
INTERNATIONAL JOURNAL OF NANOTECHNOLOGY	1475-7435	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
JOURNAL OF BIOMEDICAL NANOTECHNOLOGY	1550-7033	Nanomedicine & Nanobiotechnology	x	x	x	Y	Y	1
JOURNAL OF COMPUTATIONAL AND THEORETICAL NANOSCIENCE	1546-1955	Computational nanoscience		x	x	Y	Y	1
JOURNAL OF EXPERIMENTAL NANOSCIENCE	1745-8080	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
JOURNAL OF LASER MICRO NANOENGINEERING	1880-0688	Nanoengineering	x		x	Y	Y	1
JOURNAL OF MATERIALS CHEMISTRY A	2050-7488	Materials science (Energy)		x	x	Y	Y	0.5
JOURNAL OF MATERIALS CHEMISTRY B	2050-7518	Materials science (Medicine)		x	x	Y	Y	0.5

Title	ISSN	Thematic area	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	Scopus	Wos	Precision
		and biology)						
JOURNAL OF MATERIALS CHEMISTRY C	2050-7526	Materials science (Optic, magnetic and electronic devices)		x	x	Y	Y	0.5
JOURNAL OF MICRO-NANOLITHOGRAPHY MEMS AND MOEMS	1932-5150	Nanoengineering (Micro and nano and micro-opto electromechanical systems)	x		x	Y	Y	1
JOURNAL OF NANO RESEARCH	1662-5250	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
JOURNAL OF NANOBIO TECHNOLOGY	1477-3155	Nanobiotechnology	x	x	x	Y	Y	1
JOURNAL OF NANOELECTRONICS AND OPTOELECTRONICS	1555-130X	Nanophotonics	x	x	x	Y	Y	1
JOURNAL OF NANOMATERIALS	1687-4110	Nanomaterials	x	x	x	Y	Y	1
JOURNAL OF NANOPARTICLE RESEARCH	1388-0764	Nanoparticles	x	x	x	Y	Y	1
JOURNAL OF NANOPHOTONICS	1934-2608	Nanophotonics	x	x	x	Y	Y	1
JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY	1533-4880	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
JOURNAL OF PHYSICAL CHEMISTRY C	1932-7447	Nanochemistry (Physical chemistry)	x	x	x	Y	Y	1
JOURNAL OF PHYSICAL CHEMISTRY LETTERS	1948-7185	Chemistry (Physical chemistry)	x	x		Y	Y	1
JOURNAL OF VACUUM SCIENCE & TECHNOLOGY B	2166-2746	Nanophysics	x		x	Y	Y	1
MATERIALS EXPRESS	2158-5849	Nanomaterials	x	x		Y	Y	1
MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING	0921-5093	Materials science (Nanomaterials)	x		x	Y	Y	1
MICRO & NANO LETTERS	1750-0443	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
MICROFLUIDICS AND NANOFUIDICS	1613-4982	Nanofluidics	x		x	Y	Y	1
MICROSYSTEM TECHNOLOGIES-MICRO- AND NANOSYSTEMS-INFORMATION STORAGE AND PROCESSING SYSTEMS	0946-7076	Nanoengineering	x		x	Y	Y	1
NANO	1793-2920	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
NANO COMMUNICATION NETWORKS	1878-7789	Nanoscale communication and networking	x	x	x	Y	Y	1
NANO ENERGY	2211-2855	Nanoenergy	x	x	x	Y	Y	1
NANO LETTERS	1530-6984	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
NANO RESEARCH	1998-0124	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
NANO TODAY	1748-0132	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
NANO-MICRO LETTERS	2150-5551	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
NANOMATERIALS	2079-4991	Nanomaterials	x	x	x	N	Y	1
NANOMATERIALS AND NANOTECHNOLOGY	1847-9804	Nanomaterials	x	x	x	Y	Y	1
NANOMEDICINE	1743-5889	Nanomedicine	x	x	x	Y	Y	1



Title	ISSN	Thematic area	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	Scopus	Wos	Precision
NANOMEDICINE-NANOTECHNOLOGY BIOLOGY AND MEDICINE	1549-9634	Nanomedicine & Nanobiotechnology	x		x	Y	Y	1
NANOPHOTONICS	2192-8614	Nanophotonics	x	x	x	Y	Y	1
NANOSCALE	2040-3364	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
NANOSCALE AND MICROSCALE THERMOPHYSICAL ENGINEERING	1556-7265	Nanoengineering	x		x	Y	Y	1
NANOSCALE RESEARCH LETTERS	1931-7573	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
NANOSCIENCE AND NANOTECHNOLOGY LETTERS	1941-4900	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
NANOTECHNOLOGY	0957-4484	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
NANOTECHNOLOGY REVIEWS	2191-9089	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
NANOTOXICOLOGY	1743-5390	Nanotoxicology	x	x	x	Y	Y	1
NATURE NANOTECHNOLOGY	1748-3387	Nanoscience & Nanotechnology	x	x	x	Y	Y	1
PARTICLE & PARTICLE SYSTEMS CHARACTERIZATION	0934-0866	Nanoparticles	x	x		Y	Y	1
PHOTONICS AND NANOSTRUCTURES-FUNDAMENTALS AND APPLICATIONS	1569-4410	Nanophotonics	x		x	Y	Y	1
PHYSICA E-LOW-DIMENSIONAL SYSTEMS & NANOSTRUCTURES	1386-9477	Nanomaterials	x	x	x	Y	Y	1
PLASMONICS	1557-1955	Nanophotonics	x	x		Y	Y	1
PRECISION ENGINEERING-JOURNAL OF THE INTERNATIONAL SOCIETIES FOR PRECISION ENGINEERING AND NANOTECHNOLOGY	0141-6359	Nanoengineering	x		x	Y	Y	1
RECENT PATENTS ON NANOTECHNOLOGY	1872-2105	Nanopatens	x	x	x	Y	Y	1
SMALL	1613-6810	Nanoscience & Nanotechnology	x	x		Y	Y	1
WILEY INTERDISCIPLINARY REVIEWS-NANOMEDICINE AND NANOBIOTECHNOLOGY	1939-0041	Nanomedicine & Nanobiotechnology	x	x	x	Y	Y	1

x = Intersection (covered by the approach)

Y = Included

N = No included

### Appendix 7. Journals with null intersection

Title	ISSN	Thematic area	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	Scopus	Wos	Precision
2D MATERIALS	2053-1583	Nanomaterials (2D materials)		x		Y	Y	0.5
ACM JOURNAL ON EMERGING TECHNOLOGIES IN COMPUTING SYSTEMS	1550-4832	Computational nanoscience	x			Y	Y	1
ACS ENERGY LETTERS	2380-8195	Energy	x			N	Y	0.5
ACS SENSORS	2379-	Sensor science	x			N	Y	0

Title	ISSN	Thematic area	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	Scopus	Wos	Precision
	3694							
ACTA MATERIALIA	1359-6454	Materials science			x	Y	Y	0.5
ADVANCED ELECTRONIC MATERIALS	2199-160X	Materials science	x			Y	Y	0
ADVANCED ENERGY MATERIALS	1614-6832	Materials science (Energy)		x		Y	Y	0.5
ADVANCED FUNCTIONAL MATERIALS	1616-301X	Materials science	x			Y	Y	0.5
ADVANCED HEALTHCARE MATERIALS	2192-2640	Materials science	x			Y	Y	0
ADVANCED MATERIALS INTERFACES	2196-7350	Materials science		x		Y	Y	0.5
ADVANCED OPTICAL MATERIALS	2195-1071	Material science / Optical science		x		Y	Y	0.5
AIP ADVANCES	2158-3226	Physics	x			Y	Y	0
ANALYTICAL CHEMISTRY	0003-2700	Chemistry			x	Y	Y	0
ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	1433-7851	Physics			x	Y	Y	0
APL MATERIALS	2166-532X	Material science (Nanomaterials)	x			Y	Y	1
APPLIED PHYSICS LETTERS	0003-6951	Physics			x	Y	Y	0.5
ARTIFICIAL CELLS NANOMEDICINE AND BIOTECHNOLOGY	2169-1401	Nanomedicine & Nanobiotechnology			x	Y	Y	1
BIOINSPIRED BIOMIMETIC AND NANOBOMATERIALS	2045-9858	Nanomaterials			x	Y	Y	1
BIOMATERIALS	0142-9612	Materials science			x	Y	Y	1
BIOMEDICAL MICRODEVICES	1387-2176	Nanoengineering (Biomedical Micro/Nano electromechanical systems)	x			Y	Y	0.5
BIOMICROFLUIDICS	1932-1058	Micro and nanofluidics	x			Y	Y	0.5
BIOSENSORS & BIOELECTRONICS	0956-5663	Sensor science (Biosensing)	x			Y	Y	0.5
CANCER NANOTECHNOLOGY	1868-6958	Nanomedicine			x	Y	N	1
CARBON	0008-6223	Carbon materials		x		Y	Y	1
CARBON LETTERS	1976-4251	Carbon materials		x		Y	Y	1
CHEMELECTROCHEM	2196-0216	Chemistry (Physical chemistry: Electrochemistry)		x		Y	Y	0.5
CHEMICAL COMMUNICATIONS	1359-7345	Chemistry			x	Y	Y	0
CHEMICAL SOCIETY REVIEWS	0306-0012	Chemistry			x	Y	Y	0
CHEMISTRY OF MATERIALS	0897-4756	Chemistry			x	Y	Y	0
CONTRAST MEDIA & MOLECULAR IMAGING	1555-4309	Biochemistry (Molecular biology: Magnetizing Resonance Imaging)		x		Y	Y	1
DIAMOND AND RELATED	0925-	Carbon materials		x		Y	Y	1

Title	ISSN	Thematic area	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	Scopus	Wos	Precision
MATERIALS	9635							
E JOURNAL OF SURFACE SCIENCE AND NANOTECHNOLOGY	1348-0391	Materials science			x	Y	N	1
ELECTROCHEMISTRY COMMUNICATIONS	1388-2481	Chemistry (Physical chemistry: Electrochemistry)		x		Y	Y	0.5
ELECTROCHIMICA ACTA	0013-4686	Chemistry (Physical chemistry: Electrochemistry)		x		Y	Y	0
ENERGY & ENVIRONMENTAL SCIENCE	1754-5692	Environmental science (Energy)		x		Y	Y	0
ENVIRONMENTAL NANOTECHNOLOGY MONITORING AND MANAGEMENT	2215-1532	Nanoenvironment			x	Y	N	1
GOLD BULLETIN	0017-1557	Materials science (Gold)		x		Y	Y	0
IEEE NANOTECHNOLOGY MAGAZINE	1932-4510	Nanoengineering (Electronics)			x	Y	N	1
INTEGRATIVE BIOLOGY	1757-9694	Biology			x	Y	Y	0.5
INTERNATIONAL JOURNAL OF BIOMEDICAL NANOSCIENCE AND NANOTECHNOLOGY	1756-0799	Nanomedicine & Nanobiotechnology			x	Y	N	1
INTERNATIONAL JOURNAL OF NANO AND BIOMATERIALS	1752-8933	Nanomaterials			x	Y	N	1
INTERNATIONAL JOURNAL OF NANO ELECTRONICS AND MATERIALS	1985-5761	Nanoengineering (Electronics)			x	Y	N	1
INTERNATIONAL JOURNAL OF NANOMANUFACTURING	1746-9392	Nanoengineering (Manufacturing)			x	Y	N	1
INTERNATIONAL JOURNAL OF NANOPARTICLES	1753-2507	Nanoparticles			x	Y	N	1
INTERNATIONAL JOURNAL OF NANOSCIENCE	0219-581X	Nanoscience & Nanotechnology			x	Y	N	1
INTERNATIONAL JOURNAL OF SMART AND NANO MATERIALS	1947-5411	Nanomaterials			x	Y	N	1
JOURNAL OF APPLIED PHYSICS	0021-8979	Physics			x	Y	Y	0.5
JOURNAL OF BIONANOSCIENCE	1557-7910	Nanobiotechnology			x	Y	N	1
JOURNAL OF MICRO-BIO ROBOTICS	2194-6418	Engineering (Robotics)			x	Y	N	1
JOURNAL OF MICROELECTROMECHANICAL SYSTEMS	1057-7157	Nanoengineering (Micro / Nano electromechanical systems)	x			Y	Y	0
JOURNAL OF MICROMECHANICS AND MICROENGINEERING	0960-1317	Nanoengineering (Micro / Nano electromechanical systems)	x			Y	Y	1
JOURNAL OF NANO AND ELECTRONIC PHYSICS	2077-6772	Nanoengineering (Electronics)			x	Y	N	1
JOURNAL OF NANOMECHANICS AND MICROMECHANICS	2153-5434	Nanoengineering (Mechanics)			x	Y	N	1
JOURNAL OF NANOMEDICINE AND NANOTECHNOLOGY	2157-7439	Nanomedicine			x	Y	N	1
JOURNAL OF NANOTECHNOLOGY	1687-9503	Nanoscience & Nanotechnology			x	Y	N	1
JOURNAL OF PHYSICAL CHEMISTRY B	1520-6106	Chemistry (Physical Chemistry)			x	Y	Y	0
JOURNAL OF SOLID STATE	1432-	Chemistry (Physical		x		Y	Y	0

Title	ISSN	Thematic area	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	Scopus	Wos	Precision
ELECTROCHEMISTRY	8488	chemistry: (Electrochemistry)						
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	0002-7863	Chemistry			x	Y	Y	0
LAB ON A CHIP	1473-0197	Chemistry (Micro and nano electromechanical systems - Lab on a chip)	x			Y	Y	1
LANGMUIR	0743-7463	Chemistry			x	Y	Y	0.5
MACROMOLECULES	0024-9297	Chemistry (Polymer chemistry - Macromolecules)			x	Y	Y	0.5
MATERIALS RESEARCH EXPRESS	2053-1591	Materials science (Nanomaterials)		x		Y	Y	1
MICRO AND NANOSYSTEMS	1876-4029	Nanoengineering (Micro / Nano electromechanical systems)			x	Y	N	1
MICROELECTRONIC ENGINEERING	0167-9317	Nanoengineering (Micro / Nano electromechanical systems)	x			Y	Y	1
MICROELECTRONICS JOURNAL	0959-8324	Nanoengineering (Microelectromechanical systems)	x			Y	Y	0
MICROELECTRONICS RELIABILITY	0026-2714	Nanoengineering (Micro and nano electromechanical systems)	x			Y	Y	0
MICROMACHINES	2072-666X	Nanoengineering (Micro and nano electromechanical systems)	x			Y	Y	1
MICROPOROUS AND MESOPOROUS MATERIALS	1387-1811	Porous materials (Nanoscale porous)	x			Y	Y	1
NAMI JISHU YU JINGMI GONGCHENG NANOTECHNOLOGY AND PRECISION ENGINEERING	1672-6030	Nanoengineering			x	Y	N	1
NANO BIOMEDICINE	1883-5198	Nanomedicine & Nanobiotechnology			x	Y	N	1
NANO BIOMEDICINE AND ENGINEERING	2150-5578	Nanomedicine & Nanobiotechnology			x	Y	N	1
NANO LIFE	1793-9844	Nanomedicine & Nanobiotechnology			x	Y	N	1
NANO STRUCTURES AND NANO OBJECTS	2352-507X	Chemistry (Physical Chemistry)			x	Y	N	1
NANOETHICS	1871-4757	Nanoethics			x	Y	Y	1
NANOIMPACT	2452-0748	Nanotoxicology			x	Y	N	1
NANOSCIENCE AND NANOTECHNOLOGY ASIA	2210-6812	Nanoscience & Nanotechnology			x	Y	N	1
NANOSCIENCE AND TECHNOLOGY: AN INTERNATIONAL JOURNAL (INTERNATIONAL JOURNAL OF NANOMECHANICS SCIENCE AND TECHNOLOGY)	2572-4258	Nanoengineering (Micro and nano electromechanical systems)			x	Y	N	1
NANOTECHNOLOGIES IN RUSSIA	1995-0780	Nanoscience & Nanotechnology			x	Y	N	1
NANOTECHNOLOGY PERCEPTIONS	1660-6795	Nanoscience & Nanotechnology			x	Y	N	1

Title	ISSN	Thematic area	A <sub>1</sub>	A <sub>2</sub>	A <sub>3</sub>	Scopus	Wos	Precision
NANOTECHNOLOGY SCIENCE AND APPLICATIONS	1177-8903	Nanoscience & Nanotechnology			x	Y	N	1
NEW CARBON MATERIALS	1872-5805	Carbon materials		x		Y	Y	1
NPG ASIA MATERIALS	1884-4049	Materials science		x		Y	Y	0.5
OPENNANO	2352-9520	Nanobiology (Nanopharmacology)			x	Y	N	1
PARTICLE AND FIBRE TOXICOLOGY	1743-8977	Toxicology		x		Y	Y	0.5
PHYSICA STATUS SOLIDI B-BASIC SOLID STATE PHYSICS	0370-1972	Physics (Condensed matter & Materials physics)		x		Y	Y	0.5
PHYSICA STATUS SOLIDI-RAPID RESEARCH LETTERS	1862-6254	Physics (Condensed matter & Materials physics)		x		Y	Y	0.5
PHYSICAL REVIEW B	1098-0121	Physics (Condensed matter & Materials physics)			x	Y	Y	0.5
PHYSICAL REVIEW LETTERS	0031-9007	Physics			x	Y	Y	0
PROCEEDINGS OF THE INSTITUTION OF MECHANICAL ENGINEERS, PART N: JOURNAL OF NANOMATERIALS, NANOENGINEERING AND NANOSYSTEMS	1740-3499	Nanoengineering (Mechanical engineering)			x	Y	N	1
REVIEWS ON ADVANCED MATERIALS SCIENCE	1605-8127	Materials science (Nanomaterials)	x			Y	Y	0.5
SCIENCE OF ADVANCED MATERIALS	1947-2935	Materials science	x			Y	Y	0.5
SCRIPTA MATERIALIA	1359-6462	Materials science	x			Y	Y	0
SUPERLATTICES AND MICROSTRUCTURES	0749-6036	Materials science (Nanomaterials)		x		Y	Y	0.5

x = Covered by the approach

Y = Included

N = No included

## Appendix 8. Questionnaire

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
<p>Today, M., Hagihara, K., Kishida, K., Inui, H., &amp; Nakano, T. (2016). Microstructure and fracture toughness in boron added NbSi<sub>2</sub> (C40)/MoSi<sub>2</sub> (C11 b) duplex crystals. <i>Scripta Materialia</i>, 113(1), 236-240. doi: 10.1016/j.scriptamat.2015.11.004</p>	<p>The effect of B-addition on the microstructure and fracture toughness of (Mo<sub>0.85</sub>Nb<sub>0.15</sub>)Si<sub>2</sub> crystals with an oriented lamellar microstructure was investigated. B-addition led to an increase in the volume fraction of the C<sub>ub</sub> phase, which possesses different orientation relationship from that of the fine lamellae, and a reduction in their precipitation rate. The fracture toughness of the B-added crystal with the varied microstructure exhibited a value more than 4.0 MPa m<sup>1/2</sup>, that was significantly higher than that of the ternary crystal.</p>	<p>Transition metal silicides; Lamellar structure; Toughness; Microstructure</p>	<p>plastic-deformation behavior; mosi2 single-crystals; mechanical-properties; oriented lamellae; phase-field; silicides; composite; segregation; improvement; elements</p>			
<p>Howell, S. L., Padalkar, S., Yoon, K., Li, Q., Koleske, D. D., Wierer, J. J., Wang, G. T., &amp; Lauhon, L. J. (2013). Spatial mapping of efficiency of GaN/InGaN nanowire array solar cells using scanning photocurrent microscopy. <i>Nano Letters</i>, 13(11), 5123-5128. doi: 10.1021/nl402331u</p>	<p>GaN-InGaN core shell nanowire array devices are characterized by spectrally resolved scanning photocurrent microscopy (SPCM). The spatially resolved external quantum efficiency is correlated with structure and composition inferred from atomic force microscope (AFM) topography, scanning transmission electron microscope (STEM) imaging, Raman microspectroscopy, and scanning photocurrent microscopy (SPCM) maps of the effective absorption edge. The experimental analyses are coupled with finite difference time domain simulations to provide mechanistic understanding of spatial variations in carrier generation and collection, which is essential to the development of heterogeneous novel architecture solar cell devices.</p>	<p>Nanowire; InGaN; SPCM; solar cell; photovoltaics</p>	<p>multiple-quantum-wells; light-emitting-diodes; raman-scattering; photovoltaics; devices; nanorod</p>			
<p>Yang, P., Xu, R., Nanita, S. C., &amp; Cooks, R. G. (2006). Thermal formation of homochiral serine clusters and implications for the origin of homochirality. <i>Journal of the American Chemical Society</i>, 128(51), 17074-17086. doi: 10.1021/ja064617d</p>	<p>Spontaneous assembly of amino acids into vapor-phase clusters occurs on heating the solid compounds in air. In comparison to the other amino acids, serine forms clusters to an unusual extent, showing a magic number octamer on sublimation; this octamer can be ionized and characterized by mass spectrometry. Two isomers of the vapor-phase serine octamer are generated, the minor one at 130 degrees C and the major at 220 degrees C. The higher temperature cluster shows a strong homochiral preference, as confirmed by isotopic labeling experiments. This serine cluster, like that generated earlier from solution in electrospray ionization experiments, undergoes gas-phase enantioselective substitution reactions with other amino acids. These reactions transfer the chirality of serine to the other amino acid through enantioselective incorporation into the octamer. Other serine pyrolysis products include alanine, glycine, ethanolamine, and small dipeptides, and many of these, too, are observed to be incorporated into the thermally formed serine octamers. Chiral chromatographic analysis confirmed that L-serine sublimation produced DL-alanine, glycine, and ethanolamine, while in the presence of hydrogen sulfide, L-serine yielded L-cysteine. The data demonstrate that sublimation of serine under relatively mild conditions yields chirally enriched serine octamers and that the chiral preference of the starting serine can be transferred to other compounds through cluster-forming chemical reactions.</p>		<p>ionization mass-spectrometry; sonic spray ionization; magic number clusters; phase h/d exchange; gas-phase; electrospray-ionization; amino-acids; supramolecular chirality; structure elucidation; octamer</p>			

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Bergman, L., Rosenholm, J., Öst, A. B., Duchanoy, A., Kankaanpää, P., Heino, J., & Lindén, M. (2008). On the complexity of electrostatic suspension stabilization of functionalized silica nanoparticles for biotargeting and imaging applications. <i>Journal of Nanomaterials</i> , 2008. doi: 10.1155/2008/712514	Different means of attaching streptavidin to surface functionalized silica particles with a diameter of 240 nm were investigated with special focus on suspension stability for electrostatically stabilized suspensions. The influence of two different fluorescent dyes covalently linked to the streptavidin on suspension stability was also studied. The results clearly show that the stability of the suspensions is crucially dependent on all functional groups present on the surface. The surface functions may either directly affect the effective surface charge if the functions contain charged groups, or indirectly by affecting the relative concentration of charged groups on the particle surface. Poly(ethyleneimine)-functionalized silica particles, where the polymer is grown by surface hyperbranching polymerization, are shown to be promising candidates for bioapplications, as the zeta-potential can remain strongly positive even under biologically relevant conditions.		gene delivery; in-vivo; surface functionalization; transfection efficiency; drug-delivery; particles; carriers; cells; polyethylenimine; glutaraldehyde			
Kanamadi, C. M., Das, B. K., Kim, C. W., Cha, H. G., Ji, E. S., Kang, D. I., Jadhav, A. P., & Kang, Y. S. (2009). Template assisted growth of cobalt ferrite nanowires. <i>Journal of Nanoscience and Nanotechnology</i> , 9(8), 4942-4947. doi: 10.1166/jnn.2009.1271	Cobalt ferrite nanowires with a diameter of about 30 nm have been prepared inside anodized aluminum oxide (AAO) templates with one end closed nanopores using a vacuum infiltration method. The ferrite phase formation was confirmed by X-ray diffraction. Field emission scanning electron microscopy (FE-SEM) and transmission electron microscopy (TEM) were employed to characterize the morphology and structure of nanowires. SQUID magnetometer measurement showed that the nanowires to have both ferrimagnetic and superparamagnetic characteristics. A model for formation of discontinuous nanowires and particle agglomeration inside the template is discussed to explain these results.	Anodized Aluminum Oxide; AAO; Nanowires; Ferrite; Ferrimagnetic	magnetic-properties; anodic alumina; beta-feooh; thin-films; arrays; nanostructures; nanoparticles; fabrication; behavior; nanotubes			
Fang, L., & Li, W. J. (2012). Hydrothermal synthesis of flake-like MnCO <sub>3</sub> film under high gravity field and their thermal conversion to hierarchical Mn <sub>3</sub> O <sub>4</sub> . <i>Micro &amp; Nano Letters</i> , 7(4), 353-356. doi: 10.1049/mnl.2011.0530	A flake-like MnCO <sub>3</sub> film has been successfully synthesised by the hydrothermal method, with high gravity field using 0.5 mol/L MnCl <sub>2</sub> and 5 mol/L CO(NH) <sub>2</sub> as precursor at 120 degrees C for 30 min in the aqueous solution-bromobenzene system. The effects of the relative centrifugal field and the reaction temperature on the formation of flake-like MnCO <sub>3</sub> film were examined. The resultant samples were characterised by X-ray diffraction, Fourier transform infrared, FE-scanning electron microscopy and thermogravimetric differential thermal analysis. The results reveal that low temperature and high gravity field are favourable for the formation of flake-like MnCO <sub>3</sub> film. The hierarchical Mn <sub>3</sub> O <sub>4</sub> were obtained after calcinations of the flake-like MnCO <sub>3</sub> film at 700 degrees C for 1 h in air.		rechargeable lithium batteries; manganese carbonate; metal carbonate; ionic liquid; nanocrystals; mn(oh)(2); system; route			

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Gonzalez, J. (2008). Kohn-Luttinger superconductivity in graphene. <i>Physical Review B</i> , 78(20), 205431. doi: 10.1103/PhysRevB.78.205431	We investigate the development of superconductivity in graphene when the Fermi level becomes close to one of the Van Hove singularities of the electron system. The origin of the pairing instability lies in the strong anisotropy of the e-e scattering at the Van Hove filling, which leads to a channel with attractive coupling when making the projection of the BCS vertex on the symmetry modes with nontrivial angular dependence along the Fermi line. We show that the scale of the superconducting instability may be pushed up to temperatures larger than 10 K, depending on the ability to tune the system to the proximity of the Van Hove singularity.		renormalization-group approach; 2 dimensions; fermions			
Xiang, C., Yang, Y., & Penner, R. M. (2009). Cheating the diffraction limit: electrodeposited nanowires patterned by photolithography. <i>Chemical Communications</i> , (8), 859-873. doi: 10.1039/b815603d	The diffraction limit, $d \approx \lambda/2$ , constrains the resolution with which structures may be produced using photolithography. Practical limits for $d$ are in the 100 nm range. To circumvent this limit, photolithography can be used to fabricate a sacrificial electrode that is then used to initiate and propagate the growth by electrodeposition of a nanowire. We have described a version of this strategy in which the sacrificial electrode delimits one edge of the nascent nanowire, and a microfabricated "ceiling" constrains its height during growth. The width of the nanowire is determined by the electrochemical deposition parameters (deposition time, applied potential, and solution composition). Using this method, called lithographically patterned nanowire electrodeposition (LPNE), nanowires with minimum dimensions of 11 nm (w) x 5 nm (h) have been obtained. The lengths of these nanowires can be wafer-scale. LPNE has been used to synthesize nanowires composed of bismuth, gold, silver, palladium, platinum, and lead telluride.		conducting polymer nanowires; step-edge decoration; field-effect transistors; light-emitting diode; quartz-crystal microbalance; telluride $\text{Bi}_2\text{Te}_3$ nanowires; tin oxide nanowires; silicon nanowires; transport-properties; bismuth nanowires			
Sumesh, C. K., Patel, K. D., Pathak, V. M., & Srivastava, R. (2008). Twofold conduction mechanisms in molybdenum diselenide single crystals in the wide temperature range of 300K to 12K. <i>Chalcogenide Letters</i> , 5(8), 177-180.	Molybdenum dichalcogenides, a member of VIA-VIB transition metal dichalcogenides has been looked as a potential semiconducting material for electronic devices. This paper reports temperature variation of (12K - 300K) electrical conductivity and carrier concentration in semiconducting crystals grown by direct vapor transport technique. It is found that the conductivity behavior is extrinsic in character with three different values of activation energy in the investigated temperature range. This behavior seems to be originating from presence of defects incorporated during growth and can be explained in the frame of a model consisting of one donor level along with one shallow acceptor level.	EDAX; A1 XRD; Growth from vapour; MoSe2 single crystals; Low temperature transport properties				



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Westenfelder, B., Meyer, J. C., Biskupek, J., Kurasch, S., Scholz, F., Krill III, C. E., & Kaiser, U. (2011). Transformations of carbon adsorbates on graphene substrates under extreme heat. <i>Nano Letters</i> , 11(12), 5123-5127. doi: 10.1021/nl203224z	We describe new phenomena of structural reorganization of carbon adsorbates as revealed by in situ atomic-resolution transmission electron microscopy (TEM) performed on specimens at extreme temperatures. In our investigations, a graphene sheet serves as both a quasi-transparent substrate for TEM and as an in situ heater. The melting of gold nanoislands deposited on the substrate surface is used to evaluate the local temperature profile. At annealing temperatures around 1000 K, we observe the transformation of physisorbed hydrocarbon adsorbates into amorphous carbon monolayers and the initiation of crystallization. At temperatures exceeding 2000 K the transformation terminates in the formation of a completely polycrystalline graphene state. The resulting layers are bounded by free edges primarily in the armchair configuration.	Transmission electron microscopy; in situ Joule heating; graphene; graphene edges	in-situ observation; electron-microscopy; gold particles; temperature; aberration; atoms; edge; nanostructures; spectroscopy; stability			
Sherman, E. Y., Ban, Y., Gulyaev, L. V., & Khomitsky, D. V. (2012). Spin Tunneling and Manipulation in Nanostructures. <i>Journal of nanoscience and nanotechnology</i> , 12(9), 7535-7539. doi: 10.1166/jnn.2012.6554	The results for joint effects of tunneling and spin-orbit coupling on spin dynamics in nanostructures are presented for systems with discrete and continuous spectra. We demonstrate that tunneling plays the crucial role in the spin dynamics and the abilities of spin manipulation by external electric field. This result can be important for design of nanostructures-based spintronics devices.	Spin Dynamic; Spin-Orbit Coupling; Tunneling	single-electron spin; traversal time; transport			
Shao Z. Q., Chen, J. W., Li Y. Q., & Pan, X.Y. (2014). Thermodynamical properties of a three-dimensional free electron gas confined in a one-dimensional harmonical potential. <i>Acta Physica Sinica</i> , 63(24). doi: 10.7498/aps.63.240502	We study the thermodynamical properties of a noninteracting electron gas confined in one dimension by a harmonic-oscillator potential. The exact analytical expression for the thermodynamical potential is obtained by using a formula of contour integration. The magnetizations, magnetic susceptibilities, and the specific heats are then studied each as a function of the strength of the magnetic field in different regimes of the temperature and effective thickness. It is shown at low temperature, the magnetization, magnetic susceptibility, and the specific heat oscillate as the strength of the magnetic field increases. Especially, there exist two modes of oscillations for the specific heat in certain regimes of low temperature and effective thickness.	thermodynamical potential; magnetization; magnetic susceptibility; specific heat	diamagnetic susceptibility; magnetic-field; size corrections; systems; particles			

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Soylemez, S., Udum, Y. A., Kesik, M., Hizliates, C. G., Ergun, Y., & Toppare, L. (2015). Electrochemical and optical properties of a conducting polymer and its use in a novel biosensor for the detection of cholesterol. <i>Sensors and Actuators B: Chemical</i> , 212, 425-433. doi 10.1016/j.snb.2015.02.045	A simple and robust cholesterol biosensor was designed by immobilizing cholesterol oxidase (ChOx) onto a conducting polymer modified graphite electrode. For this purpose, monomer, (Z)-4-(4-(9H-carbazol-9-yl) benzylidene) 2 (4 nitrophenyl) oxazol-5(4H)-one (CBNP), was synthesized and electrochemically polymerized on an electrode to achieve an effective immobilization platform for enzyme immobilization. After electropolymerization of the monomer (CBNP), electrochemical and spectroelectrochemical properties were investigated. Through the presence of nitro group on the polymer backbone hydrogen-bonding between enzyme molecules and polymer was achieved. Moreover, strong pi-pi stacking between aromatic moieties in the polymer and aromatic residues of the enzyme enables a sensitive and reliable biosensor by conserving the crucial structure of biological molecules during the enzymatic reaction. The efficient interaction of the enzyme with the polymer coated surface brings easy and long-life detection of the substrate, cholesterol. After successful immobilization of ChOx with the help of glutaraldehyde as the crosslinking agent, amperometric biosensor responses were recorded at -0.7 V vs Ag wire in phosphate buffer (pH 7.0). K-M(app) (37.3 $\mu$ M), I-max (3.92 $\mu$ A), LOD (0.4063 $\mu$ M) and sensitivity (1.49 pA $\mu$ M <sup>-1</sup> cm <sup>-2</sup> ) values were determined. Finally, the prepared biosensor was successfully applied for determination of cholesterol content in real blood samples.	Amperometric biosensor; Polymer based biosensor; Conducting polymer; Cholesterol biosensor; Cholesterol oxidase	glassy-carbon electrode; oxidase; immobilization; film; nanotubes; graphene; network; sensor; serum			
Dyshin, A. A., Eliseeva, O. V., Bondarenko, G. V., Kolker, A. M., & Kiselev, M. G. (2016). Dispersion of single-walled carbon nanotubes in dimethylacetamide and a dimethylacetamide–cholic acid mixture. <i>Russian Journal of Physical Chemistry A</i> , 90(12), 2434-2439. doi 10.1016/j.snb.2015.02.045	A way of dispersing single-walled carbon nanotubes in preparing stable suspensions with high concentrations of individual nanotubes in amide solvents is described. The obtained suspensions are studied via Raman spectroscopy. The dependence of the degree of single-walled carbon nanotube (SWNT) dispersion in individual and mixed amide solvents on the type of solvent, the mass of nanotubes, and the concentration of cholic acid is established. A technique for processing spectral data to estimate the diameters and chiralities of individual nanotubes in suspension is described in detail.	dimethyl acetamide; cholic acid; dispersing nanotubes; single-walled carbon nanotubes; SWNT suspensions; Raman spectroscopy; decomposition of spectra; calculating SWNT diameters; estimating chirality	dissolution; dynamics			

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
Dechow, J., Forchel, A., Lanz, T., & Haase, A. (2000). Fabrication of NMR - Microsensors for nanoliter sample volumes. <i>Microelectronic engineering</i> , 53(1), 517-519.	The fabrication of micro-sensors for NMR-spectroscopy on both glass and GaAs is presented. Planar coils with inner diameter from 50 $\mu\text{m}$ to 400 $\mu\text{m}$ including a coplanar wave-guide leading to the bonding pads were combined with a chamber for liquid samples of 200-500 $\mu\text{m}$ diameter on the backside of the substrate. The microcoil served as a receiver in a H-1-NMR experiment at 11T(500 MHz). In initial experiments, the spectrum of 60 nl-volumes of pure silicone-oil were detected by the microcoil.					
Hilleringmann, U., Vieregge, T., & Horstmann, J. T. (2000). A structure definition technique for 25 nm lines of silicon and related materials. <i>Microelectronic engineering</i> , 53(1-4), 569-572.	This paper describes an interesting solution to integrate features with nanometer scale on silicon without using a special lithography tool. Simple layer deposition and etching processes fulfil the lithography demands of the SIA roadmap for the year 2012. This structure definition technique has been used to generate polysilicon gates, silicon oxide and nitride, aluminum, tungsten and titanium nitride lines down to 25 nm width with excellent homogeneity over a 100 mm silicon wafer. It is transferable to any technology line, because only standard process steps like CVD deposition, dry and wet etching, and conventional optical lithography are necessary.					
Chong, Y. M., Leung, K. M., Ma, K. L., Zhang, W. J., Bello, I., & Lee, S. T. (2006). Growing cubic boron nitride films at different temperatures. <i>Diamond and related materials</i> , 15(4), 1155-1160.	Cubic boron nitride (cBN) films have been synthesized by both physical and chemical vapor deposition (PVD and CVD) methods at a wide range of substrate temperature. Some works conclude that the cBN growth is insensitive to the temperature parameter while few works suggest that substrate temperature plays a considerable role at cBN deposition, furthermore, the different temperatures used for the nucleation and growth make the situation more complex. In this work, we investigated systematically the growth of cBN films on CVD diamond surfaces at variable temperatures (from 200 to 1100 degrees C) using electron cyclotron resonance microwave plasma CVD (ECR-MPCVD) and radio-frequency magnetron sputtering (RF-MS) methods. The role of substrate temperature is discussed in the view of controlling phase purity, crystallinity, growth rate, and residual stress of cBN films deposited. Under optimized conditions, several-micrometers thick films are prepared by ECR-MPCVD as demonstrated on the example of a 3- $\mu\text{m}$ thick cBN film grown at 900 degrees C with faceted surfaces. The sizes of crystallites are fairly large (similar to 0.4 $\mu\text{m}$ ) to yield visible Raman spectra characteristic to cBN.	cubic boron nitrides; chemical vapor deposition; physical vapor deposition; fluorine chemistry	chemical-vapor-deposition; pulsed-laser deposition; cbn films; bn films; growth; diamond; plasma; quality; epitaxy; phase			

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
Lin, T., Zheng, K., Wang, C. L., & Ma, X. Y. (2007). Photoluminescence study of AlGaInP/GaInP quantum well intermixing induced by zinc impurity diffusion. <i>Journal of Crystal Growth</i> , 309(2), 140-144. doi: 10.1016/j.jcrysgro.2007.09.029	AlGaInP/GaInP quantum well intermixing phenomena induced by Zn impurity diffusion at 540 degrees C were studied using room-temperature photoluminescence (PL) spectroscopy. As the diffusion time increased from 40 to 120 min, PL blue shift taken on the AlGaInP/GaInP quantum well regions increased from 36.3 to 171.6 meV. Moreover, when the diffusion time was equal to or above 60 min, it was observed firstly that a PL red shift occurred with a PL blue shift on the samples. After detailed analysis, it was found that the red-shift PL spectra were measured on the Ga <sub>0.51</sub> In <sub>0.49</sub> P buffer layer of the samples, and the mechanism of the PL red shift and the PL blue shift were studied qualitatively.	diffusion ; metalorganic vapor phase epitaxy; semiconducting III-V material; laser diodes	low-temperature; laser-diodes; superlattices; GaAs; layer; Al			
Borysenko, K. M., Mullen, J. T., Barry, E. A., Paul, S., Semenov, Y. G., Zavada, J. M., Nardelli, M. & Kim, K. W. (2010). First-principles analysis of electron-phonon interactions in graphene. <i>Physical Review B</i> , 81(12). doi 10.1103/PhysRevB.81.121412	The electron-phonon interaction in monolayer graphene is investigated using density-functional perturbation theory. The results indicate that the electron-phonon interaction strength is of comparable magnitude for all four in-plane phonon branches and must be considered simultaneously. Moreover, the calculated scattering rates suggest an acoustic-phonon contribution that is much weaker than previously thought, revealing an important role of optical phonons even at low energies. Accordingly it is predicted, in good agreement with a recent measurement, that the intrinsic mobility of graphene may be more than an order of magnitude larger than the already high values reported in suspended samples.					
Vikram, S. V., Phase, D. M., & Chandel, V. S. (2010). High-TC phase transition in K <sub>2</sub> Ti <sub>6</sub> O <sub>13</sub> lead-free ceramic synthesised using solid-state reaction. <i>Journal of Materials Science: Materials in Electronics</i> , 21(9), 902-905. doi: 10.1007/s10854-009-0015-0	Solid-state reaction synthesised K <sub>2</sub> Ti <sub>6</sub> O <sub>13</sub> lead-free ceramic was characterized using XRD, SEM, and X-band EPR, at room temperature. EPR-spectra showed the presence of (Fe <sup>3+</sup> (Ti) - V-O(center dot center dot)) O defect associate dipoles, in orthorhombic phase, responsible for the broadening of the dielectric anomaly identified in the epsilon(r) (T) plots at T-C similar to 300 degrees C. This anomaly resembled a ferroelectric-paraelectric type phase transition following Curie-Weiss type trend. Besides, dielectric loss mechanism jointly represented electrical conduction, dipole orientation, and space charge polarization.		potassium hexatitanate; thin-films; ferroelectrics; octatitanate; whiskers; defects; matrix; Na			

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<p>Bora, D. K., Braun, A., Erni, R., Fortunato, G., Graule, T., &amp; Constable, E. C. (2011). Hydrothermal treatment of a hematite film leads to highly oriented faceted nanostructures with enhanced photocurrents. <i>Chemistry of Materials</i>, 23(8), 2051-2061. doi: 10.1021/cm102826n</p>	<p>A simple one-pot hydrothermal method is described for conveying a dipcoated hematite nano particle film into an array of nanorods with superimposed flowerlike structures suitable for water splitting in photoelectrochemical cells. The hydrothermal treatment of the dip-coated hematite film with FeCl<sub>3</sub> 6H<sub>2</sub>O and L-arginine enhances the photocurrent by a factor of 2. It has been found that hydrothermal treatment changes the optical properties of the pristine hematite film, but the energy band gap (E<sub>g</sub>) does not change significantly to show some electronic effect. X-ray diffractograms of pristine and hydrothermally modified films reveal evolution of preferential orientations and textures. Electron micrographs show that the particles are more prismatic after modification with a size of around 40nm x 200 nm. The X-ray photoelectron spectroscopy valence-band spectra point at a depletion of the spectral intensity near the Fermi energy upon hydrothermal modification. The photocurrent density of the pristine film reached 218 <math>\mu\text{A}/\text{cm}^2</math> after 48 h of hydrothermal treatment, and this increase was found to be due to the high specific surface area of the modified film and changes in the optical properties of the pristine film after hydrothermal treatment.</p>	<p>hematite thin film; photocurrent; hydrothermal treatment; faceted nanostructures; flowerlike superstructures</p>	<p>biomolecule-assisted synthesis; template-free synthesis; lithium ion battery; optical-properties; water oxidation; thin-films; alpha-fe<sub>2</sub>o<sub>3</sub> superstructures; photocatalytic properties; electronic-structure; magnetic-property</p>			
<p>Ghalamestani, S. G., Heurlin, M., Wernersson, L. E., Lehmann, S., &amp; Dick, K. A. (2012). Growth of InAs/InP core-shell nanowires with various pure crystal structures. <i>Nanotechnology</i>, 23(28), 285601. doi: 10.1088/0957-4484/23/28/285601</p>	<p>We have studied the epitaxial growth of an InP shell on various pure InAs core nanowire crystal structures by metal-organic vapor phase epitaxy. The InP shell is grown on wurtzite (WZ), zinc-blende (ZB), and {111}- and {110}-type faceted ZB twin-plane superlattice (TSL) structures by tuning the InP shell growth parameters and controlling the shell thickness. The growth results, particularly on the WZ nanowires, show that homogeneous InP shell growth is promoted at relatively high temperatures (similar to 500 degrees C), but that the InAs nanowires decompose under the applied conditions. In order to protect the InAs core nanowires from decomposition, a short protective InP segment is first grown axially at lower temperatures (420-460 degrees C), before commencing the radial growth at a higher temperature. Further studies revealed that the InP radial growth rate is significantly higher on the ZB and TSL nanowires compared to WZ counterparts, and shows a strong anisotropy in polar directions. As a result, thin shells were obtained during low temperature InP growth on ZB structures, while a higher temperature was used to obtain uniform thick shells. In addition, a schematic growth model is suggested to explain the basic processes occurring during the shell growth on the TSL crystal structures.</p>		<p>vapor-phase epitaxy; lateral growth; inp; fabrication; devices; layers</p>			

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<p>Chiacchiarelli, L. M., Rallini, M., Monti, M., Puglia, D., Kenny, J. M., &amp; Torre, L. (2013). The role of irreversible and reversible phenomena in the piezoresistive behavior of graphene epoxy nanocomposites applied to structural health monitoring. <i>Composites Science and Technology</i>, 80, 73-79. doi: 10.1016/j.compscitech.2013.03.009</p>	<p>The use of graphene for the development of a strain and damage sensor was evaluated and modeled. To achieve this, a graphene epoxy reactive mixture was used as a conductive coating which was cured onto a carbon fiber reinforced composite. This methodology proved to be very effective where substantial changes in piezoresistivity (up to 400%) were found as a function of strain (up to 2%). This contributed to a very high linear gauge factor (56.7(+/- 0.69)). The role of reversible and irreversible phenomena in the sensor piezoresistivity was modeled using the concepts of tunneling currents and conduction paths. In order to predict the response at higher deformation, an irreversible component was introduced to account for the substantial increase of piezoresistivity. A model which incorporated both components was able to predict the piezoresistivity up to high deformation.</p>	<p>Nano composites; Polymer-matrix properties; Electrical Properties; Modeling</p>	<p>fiber-reinforced composites; carbon nanotubes; electrical-properties; damage; nanofibers; strain; dispersion; matrix; rods</p>			
<p>Park, S., Lee, J., Do, I. G., Jang, J., Rho, K., Ahn, S., Maruja, L., Kim S. J., Kim, K. M., Mao, M., Oh, E., Kim, Y. J., Kim, J., &amp; Choi, Y. L. (2014). Aberrant CDK4 amplification in refractory rhabdomyosarcoma as identified by genomic profiling. <i>Scientific reports</i>, 4, 3623. doi: 10.1038/srep03623</p>	<p>Rhabdomyosarcoma (RMS) is the most commonly occurring type of soft tissue tumor in children. However, it is rare in adults, and therefore, very little is known about the most appropriate treatment strategy for adult RMS patients. We performed genomic analysis of RMS cells derived from a 27-year-old male patient whose disease was refractory to treatment. A peritoneal seeding nodule from the primary tumor, pleural metastases, malignant pleural effusion, and ascites obtained during disease progression, were analyzed. Whole exome sequencing revealed 23 candidate variants, and 10 of 23 mutations were validated by Sanger sequencing. Three of 10 mutations were present in both primary and metastatic tumors, and 3 mutations were detected only in metastatic specimens. Comparative genomic hybridization array analysis revealed prominent amplification in the 12q13-14 region, and more specifically, the CDK4 proto-oncogene was highly amplified. ALK overexpression was observed at both protein and RNA levels. However, an ALK fusion assay using NanoString technology failed to show any ALK rearrangements. Little genetic heterogeneity was observed between primary and metastatic RMS cells. We propose that CDK4, located at 12q14, is a potential target for drug development for RMS treatment.</p>		<p>childrens oncology group; prognostic-factors; intergroup-rhabdomyosarcoma; metastatic rhabdomyosarcoma; adult rhabdomyosarcoma; gene-expression; nonmetastatic rhabdomyosarcoma; dedifferentiated liposarcoma; alveolar rhabdomyosarcoma; cancer</p>			

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
Foos, E. E., Yoon, W., Lumb, M. P., Tischler, J. G., & Townsend, T. K. (2013). Inorganic photovoltaic devices fabricated using nanocrystal spray deposition. <i>ACS applied materials &amp; interfaces</i> , 5(18), 8828-8832. doi: 10.1021/am402423f	Soluble inorganic nanocrystals offer a potential route to the fabrication of all-inorganic devices using solution deposition techniques. Spray processing offers several advantages over the more common spin- and dip-coating procedures, including reduced material loss during fabrication, higher sample throughput, and deposition over a larger area. The primary difference observed, however, is an overall increase in the film roughness. In an attempt to quantify the impact of this morphology change on the devices, we compare the overall performance of spray-deposited versus spin-coated CdTe-based Schottky junction solar cells and model their dark current-voltage characteristics. Spray deposition of the active layer results in a power conversion efficiency of 2.3 +/- 0.3% with a fill factor of 45.7 +/- 3.4%, V-oc of 0.39 +/- 0.06 V, and J(sc) of 13.3 +/- 3.0 mA/cm(2) under one sun illumination.	photovoltaic; nanocrystal; processing; CdTe; spray; modeling	colloidal quantum dots; solar-cells; films; cdse; cdte			
Gu, J., Xiao, P., Huang, Y., Zhang, J., & Chen, T. (2015). Controlled functionalization of carbon nanotubes as superhydrophobic material for adjustable oil/water separation. <i>Journal of Materials Chemistry A</i> , 3(8), 4124-4128. doi: 10.1039/c4ta07173e	A robust strategy for fabricating superhydrophobic carbon nanotube (CNT)-based hybrid materials as a separation membrane through the covalent attachment of the fluorine-bearing organosilane 1H,1H,2H,2H-perfluorodecyltriethoxysilane (PFDTs) onto -OH functionalized CNTs is proposed. This method resulted in PFDTs/CNT superhydrophobic materials with controlled functionalization that could be used to effectively separate various surfactant-stabilized water-in-oil emulsions with high separation efficiency and high flux. It maintains stable superhydrophobicity and high separation efficiency under extreme conditions, including high or low temperature and strongly acidic or alkaline solutions, and shows fire-retardant properties.		organic-solvents; surfaces; films; graphene; oils; fabrication; removal; sensors; water			
Yin, Z., Zheng, Q., Chen, S. C., Li, J., Cai, D., Ma, Y., & Wei, J. (2015). Solution-derived poly(ethylene glycol)-TiO <sub>x</sub> nanocomposite film as a universal cathode buffer layer for enhancing efficiency and stability of polymer solar cells. <i>Nano Research</i> , 8(2), 456-468. doi: 10.1007/s12274-014-0615-8	Highly efficient and stable polymer solar cells (PSCs) have been fabricated by adopting solution-derived hybrid poly(ethylene glycol)-titanium oxide (PEG-TiO (x) ) nanocomposite films as a novel and universal cathode buffer layer (CBL), which can greatly improve device performance by reducing interface energy barriers and enhancing charge extraction/collection. The performance of inverted PSCs with varied bulk-heterojunctions (BHJs) based on this hybrid nanocomposite CBL was found to be much better than those of control devices with a pure TiO (x) CBL or without a CBL. An excellent power conversion efficiency up to 9.05% under AM 1.5G irradiation (100 mW center dot cm(-2)) was demonstrated, which represents a record high value for inverted PSCs with TiO (x) -based interface materials.	titanium oxide; nanocomposites; energy conversion; organic solar cells; interface engineering; device stability	power conversion efficiency; electron-transport layer; high-performance; titanium-oxide; composite film; thin-films; tio2; tandem; transparent; interlayer			

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
Meng, D., Wang, G., San, X., Shen, Y., Zhao, G., Zhang, Y., & Meng, F. (2015). CTAB-assisted hydrothermal synthesis of WO <sub>3</sub> hierarchical porous structures and investigation of their sensing properties. <i>Journal of Nanomaterials</i> , 16(1), 364. doi: 10.1155/2015/393205	WO <sub>3</sub> hierarchical porous structures were successfully synthesized via cetyltrimethylammonium bromide-(CTAB-) assisted hydrothermal method. The structure and morphology were investigated using scanning electron microscope, X-ray diffractometer, transmission electron microscopy, X-ray photoelectron spectra, Brunauer-Emmett-Teller nitrogen adsorption-desorption, and thermogravimetry and differential thermal analysis. The result demonstrated that WO <sub>3</sub> hierarchical porous structures with an orthorhombic structure were constructed by a number of nanoparticles about 50-100 nm in diameters. The H <sub>2</sub> gas sensing measurements showed that well-defined WO <sub>3</sub> hierarchical porous structures with a large specific surface area exhibited the higher sensitivity compared with products without CTAB at all operating temperatures. Moreover, the reversible and fast response to H <sub>2</sub> gas and good selectivity were obtained. The results indicated that the WO <sub>3</sub> hierarchical porous structures are promising materials for gas sensors.		ion batteries; solar-cells; gas; film; nanostructures; nanoparticles; mechanism; oxide			
Gong, J., & Wilkinson, A. J. (2016). Sample size effects on grain boundary sliding. <i>Scripta Materialia</i> , 114, 17-20. doi: 10.1016/j.scriptamat.2015.11.029	Grain boundary sliding is an important deformation mechanism that contributes to creep and superplastic forming. In tin-based lead-free solders grain boundary sliding can make significant contributions to in service performance. Novel micro-compression tests designed to isolate individual grain boundaries and assess their mechanical resistance to sliding were conducted on tin. The boundary sliding deformation was more obvious for smaller sample cross-sections and made a larger contribution to the overall deformation. As with dislocation and twinning mediated plasticity there was a significant size effect in which the resistance to grain boundary sliding increases as the sample size is reduced.	Grain boundary sliding; Tin; Micromechanics	mechanical-properties; fracture-toughness; solder joints; micron scale; copper; plasticity; crystal; deformation; strength; aluminum			
Hu, D., Wang, H. Y., & Zhu, Q. F. (2016). Design of an ultra-broadband and polarization-insensitive solar absorber using a circular-shaped ring resonator. <i>Journal of Nanophotonics</i> , 10(2). doi: 10.1117/1.JNP.10.026021	An ultra-broadband and polarization-independent metamaterial absorber consisting of a chromium circular-shaped ring resonator embedded in a dielectric layer and a chromium ground plane is numerically investigated in the solar spectrum. Simulation results show that the absorber can obtain the average absorption of 95.5% over most the solar spectrum, near-infrared, and short-wavelength infrared regime (400 to 2500 nm). The absorption mechanism of the ultra-broadband metamaterial absorber originates from the overlapping of two different resonance wavelengths. In particular, the electromagnetic energy is almost completely dissipated in the chromium layer, which makes it independent on the loss of the dielectric layer and widens the range of choices for potential dielectric materials. Our designed absorber has high practical feasibility and appears to be very promising for solar energy harvesting, thermal imaging, and emissivity control applications.	broadband; polarization-independent; metamaterial; absorber	perfect absorber; light-absorption; metamaterials; cloak			



Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
Wilson, L. R., Carder, D. A., Steer, M. J., Cockburn, J. W., Hopkinson, M., Chia, C. K., ... & Airey, R. (2002). Strategies for reducing the emission wavelength of GaAs-AlAs quantum cascade lasers. <i>Physica E: Low-dimensional Systems and Nanostructures</i> , 13(2), 835-839.	We report two novel methods for reducing the emission wavelength of GaAs-AlAs quantum cascade lasers. We demonstrate that for lasing to occur electron injection into the upper laser level must proceed via Gamma states confined below the lowest X state in the injection barrier. The limit this places on the minimum operating wavelength ( $\lambda$ approximate to 8 $\mu\text{m}$ ) is overcome by utilising a novel injection barrier design to achieve lasing at $\lambda = 7.2 \mu\text{m}$ . In addition, we have deposited InAs monolayers in the active regions of a GaAs-AlAs quantum cascade laser to decrease the lasing transition wavelength, The InAs monolayers have a minimal effect on the upper laser level but decrease the confinement energy of the lower laser level. Thus a significantly reduced emission wavelength (8.3 $\mu\text{m}$ compared with 11.2 $\mu\text{m}$ ) is achieved whilst maintaining very similar laser performance.	quantum cascade laser; GaAs based; intervalley scattering	well structures; electron-transfer; operation			
Du, X., & Hlady, V. (2002). Monolayer formation on silicon and mica surfaces rearranged from N-hexadecanoyl-L-alanine supramolecular structures. <i>The Journal of Physical Chemistry B</i> , 106(29), 7295-7299. doi: 10.1021/jp0209603	The rearrangements of N-hexadecanoyl-L-alanine supramolecular structures in water to form monolayers on silicon and mica surfaces have been investigated using atomic force microscopy. It is the first time that such a monolayer with the polar groups on the solid surface and the alkyl chains up is obtained through a rational molecular design. The monolayer formation results from the strong interaction between the molecular headgroups and the surface, the intermolecular hydrogen bonding interaction via a six-membered ring structure in the case of silicon surfaces, and the additional attractive force in the case of mica surfaces. The anisotropic and dendritic growth structures, clearly observed for the monolayers rearranged on mica surfaces, are indicative of a homochiral effect. The differences in height and morphology of the monolayers on the two types of surfaces are considered to be relevant to the surface roughness and to the interactions between the molecules and the surface.		self-assembled monolayers; langmuir-blodgett-films; chiral discrimination; ftir spectroscopy; absorption-spectroscopy; fluorescence microscopy; air/water interface; infrared reflection; aqueous-solution; metal-complex			
Gotter, R., Ruocco, A., Butterfield, M. T., Iacobucci, S., Stefani, G., & Bartynski, R. A. (2003). Angle-resolved Auger-photoelectron coincidence spectroscopy (AR-APECS) of the Ge (100) surface. <i>Physical Review B</i> , 67(3), 033303. doi: 10.1103/PhysRevB.67.033303	We have measured the angular distribution of Ge L3M45M45 Auger electrons in coincidence with Ge 2p(3/2) core photoelectrons along the (001) azimuth of the Ge(100) surface. Intensity modulations arising from diffraction effects are suppressed in the coincidence Auger angular distribution and, when specific emission angles of the photoelectrons are considered, new features appear. We attribute the former effect to enhanced surface specificity of the coincidence technique and the latter to sensitivity of the coincidence measurement to alignment of the core hole state.		electron diffraction; photoionization			

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
Nicolaides, A. (2003). Singlet hydrocarbon carbenes with high barriers toward isomerization: A computational investigation. <i>Journal of the American Chemical Society</i> , 125(30), 9070-9073. doi: 10.1021/ja0299699	A prerequisite for a stable singlet hydrocarbon carbene is the existence of high barriers toward isomerization. Four derivatives of cyclopentylidene (1-4) with rigid and varying carbon cages are examined computationally at the B3LYP/6-311+G(d,p) level of theory. Singlet ground states are predicted for carbenes 1-4, with $\Delta E(\text{ST})$ 's = 7-22 kcal/mol. The rearrangement paths considered are 1,3-hydrogen shift, 1,2-carbon shift and beta-CC bond-cleavage. Carbenes 3 and 4 lie in relatively shallow potential-energy wells (around 4 and 6 kcal/mol, respectively) and are expected to rearrange via 1,3-hydrogen shifts to cyclopropane derivatives. For 1 and 2, the lowest energy rearrangement path is beta-CC bond-cleavage requiring about 12 and 20 kcal/mol, respectively, placing 2 in the deepest potential-energy well among the four carbenes.		stable carbenes; density; cyclobutylidene; cyclobutenylidene; rearrangements; migration; hydrogen; carbon; state			
Mao, C., Qi, J., & Belcher, A. M. (2003). Building Quantum Dots into Solids with Well-Defined Shapes. <i>Advanced Functional Materials</i> , 13(8), 648-656. doi: 10.1002/adfm.200304297	Quantum dots (QDs) chemically synthesized in solution at a higher temperature (85degreesC) were built in situ into a variety of three-dimensional (3D) close-packed QD ensembles (QD solids) with well-defined shapes: needles, disks, rods, spheres, bundles, stars, ribbons, and transition structures (TSs). Design strategies using a novel cold-treatment (-25 to 0degreesC) process immediately following the synthesis of the QDs provided control over these shapes, independently from the II-VI materials used. Transformation occurred between different shapes by the rearrangement of the QDs within the QD ensembles. The QD solids were characterized by advanced electron microscopy and photoluminescence spectroscopy. The cold treatment strategy is versatile and has been applied to several II-VI QDs (CdS, ZnS, and CdSe) and may be extended to other QD systems and other chemical approaches.		semiconductor nanocrystals; cdse nanocrystals; optical gain; nanoparticles; superlattices; coalescence; assemblies; ensemble; states			
Hichria, A., & Jazirib, S. (2003). Two Carriers in Vertically Coupled Quantum Dots: Magnetic Field Effect. <i>Journal of nanoscience and nanotechnology</i> , 3(3), 263-269. doi: 10.1166/jnn.2003.162	We study a two-charge-carrier (two holes or two electrons) quantum dot molecule in a magnetic field. In comparison with the electron states in the double quantum dot, the switching between the hole states is achieved by changing both the inter-dot distance and magnetic field. We use harmonic potentials to model the confining of two charge carriers and calculate the energy difference $\Delta E$ between the two lowest energy states with the Hund-Mulliken technique, including the Coulomb interaction. Introducing the Zeeman effect, we note a ground-state crossing, which can be observed as a pronounced jump in the magnetization at a perpendicular magnetic field of a few Tesla. The ground states of the molecule provide a possible realization for a quantum gate.	quantum dots; valence band mixing; harmonic Potential; Hund-Mulliken technique; switching; phase transition; qubit; magnetization	artificial atoms			

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
Bao, M., Yang, H., Sun, Y., & French, P. J. (2003). Modified Reynolds' equation and analytical analysis of squeeze-film air damping of perforated structures. <i>Journal of Micromechanics and Microengineering</i> , 13(6), 795.	We modified the Reynolds equation to extend its applications to squeeze-film air damping of perforated plates (i.e., the hole-plates) by adding a term related to the damping effect of gas flow through holes. The modified Reynolds equation (MRE) is generally effective for a perforated hole-plate with a finite thickness and finite lateral dimensions as well as a non-perforated hole-plate. Analytical expressions of damping pressure for long rectangular hole-plates and regular rectangular hole-plates have been found. For MEMS devices with typical dimensions, 'effective damping width' approximation is introduced so that the boundary effect on damping force can be treated easily. The conditions for 'effective damping width' approximation are discussed. Based on the concept of 'effective damping width', damping forces for circular plates and even hole-plates with irregular shapes can be found. The results obtained by the MIZE method match the numerical results obtained by ANSYS/FLOTRAN very well. The comparison between the MIZE results and the experimental results by Kim et al (1999 MEMS '99 pp 296-301) shows that the MIZE results agree with the experimental results much better than the FEM simulation given by Kim et al.					
Alcala, M. D., Criado, J. M., Real, C., Grygar, T., Nejezchleba, M., Subrt, J., & Petrovsky, E. (2004). Synthesis of nanocrystalline magnetite by mechanical alloying of iron and hematite. <i>Journal of Materials Science</i> , 39(7), 2365-2370.	The synthesis of magnetite has been studied by mechanical alloying in an inert atmosphere of a stoichiometric mixture of micrometric particle size iron and hematite powders. The final products have been characterised by chemical analysis, SEM, TEM, XRD, Mossbauer spectroscopy as well as specific surface and magnetic measurements. The magnetite obtained in this way exhibits a high magnetic hardness. The formation of a wustite layer on the magnetite core, because of the reaction between magnetite and iron contamination coming from the bowls and grinding balls, tends to decrease the coercive force of magnetite. The formation of this phase would be avoided by controlling the grinding time.		electrochemical dissolution; gamma-fe2o3 particles; thermal-stability; size; microparticles; nanoparticles; fabrication; voltammetry; iron(iii); evolution			
Shi, Z., Wang, Q., Ye, W., Li, Y., & Yang, Y. (2006). Synthesis and characterization of mesoporous titanium pyrophosphate as lithium intercalation electrode materials. <i>Microporous and mesoporous materials</i> , 88(1), 232-237. doi: 10.1016/j.micromeso.2005.09.013	Mesoporous titanium pyrophosphates have been synthesized by a sol-gel template method with further calcinations at or below the temperature of 700 degrees C. When calcined at 800 degrees C, crystalline TiP2O7 will be formed accompanied with the break down of meso-structure in the precursor. Mesoporous TiP2O7 shows a similar lithium ion intercalation behavior to that of solid solution in the electrochemical tests. When cycled at high charge/discharge rate, mesoporous TiP2O7 calcined at 700 degrees C delivers a higher specific discharge capacity than that of crystalline TiP2O7, indicating that mesoporous structure is beneficial for improving the transportation and intercalation/deintercalation behavior of lithium ions in the materials, thus improving the charge/discharge performance of the materials at high charge/discharge rate.	mesoporous materials; titanium pyrophosphate; cathode material; lithium ion batteries	cathode materials; ion batteries; nanostructured materials; block-copolymer; performance; progress; oxide; nanotechnology; insertion; storage			

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
Matsubara, M., Kortus, J., Parlebas, J. C., & Massobrio, C. (2006). Dynamical identification of a threshold instability in Si-doped heterofullerenes. <i>Physical Review Letters</i> , 96(15), 155502. doi: 10.1103/PhysRevLett.96.155502	We rationalize the origins of a threshold instability and the mechanism of finite temperature fragmentation in highly Si-doped C60-mSim heterofullerenes via a first-principles approach. Cage disruption is driven by enhanced fluctuations of the most internal Si atoms. These are located within fully segregated Si regions neighboring the C-populated part of the cage. The predominance of inner Si atoms over those involved in Si-C bonds marks the transition from thermally stable to unstable C60-mSim systems at m=20.		metal-fullerene clusters; molecular-dynamics; 1st principles; carbon clusters; mixed clusters; cage; density; boron			
Hájek, M., Veselý, J., & Cieslar, M. (2007). Precision of electrical resistivity measurements. <i>Materials Science and Engineering: A</i> , 462(1), 339-342. doi: 10.1016/j.msea.2006.01.175	The influence of the specimen shape on the electrical resistivity measurements was investigated both theoretically, by means of finite element method modelling, and experimentally, by measuring electrical resistivity of samples of variable shapes. Precision of electrical resistivity measurements using a four-point method for samples of arbitrary shape was critically reviewed.	electrical resistivity; four-point method; finite elements	deformation; order; al			
Stopa, M., & Marcus, C. M. (2008). Magnetic field control of exchange and noise immunity in double quantum dots. <i>Nano letters</i> , 8(6), 1778-1782. doi: 10.1021/nl801282t	We employ density functional calculated eigenstates as a basis for exact diagonalization studies of semiconductor double quantum dots, with two electrons, through the transition from the symmetric bias regime to the regime where both electrons occupy the same dot. We calculate the singlet-triplet splitting $J(\epsilon)$ as a function of bias detuning $\epsilon$ and explain its functional shape with a simple, double anticrossing model. A voltage noise suppression "sweet spot," where $dJ(\epsilon)/d\epsilon = 0$ with nonzero $J(\epsilon)$ , is predicted and shown to be tunable with a magnetic field $B$ .		coulomb-blockade; electron-spin; polarization			
Ao, Y., Xu, J., & Fu, D. (2009). Study on the effect of different acids on the structure and photocatalytic activity of mesoporous titania. <i>Applied Surface Science</i> , 256(1), 239-245. doi: 10.1016/j.apsusc.2009.08.008	Nanocrystalline mesoporous titania was synthesized via a combined sol-gel process with surfactant-assisted templating method using cetyltrimethyl ammonium bromide (CTAB) as the structure-directing agent. The process was catalyzed by different acid (hydrochloric acid, nitric acid, sulfuric acid, or phosphoric acid). The prepared samples were characterized by XRD, TEM, BET and FT-IR. The photocatalytic activity of the samples was determined by degradation of phenol in aqueous solution. Results showed that different acid had different effect on the structure and crystal phase of the samples. The sample adjusted by phosphoric acid showed highest surface area and photocatalytic activity. The formation mechanism of the samples catalyzed by different acid was also discussed.	Mesoporous structure; Titania; Sol-gel; Mechanism; Photocatalysis	visible-light irradiation; tio2 particles; sol; degradation; adsorption; nanocrystallites; silica; films; oxide			
Kher, S., Dixit, A., Rawat, D. N., & Sodha, M. S. (2010). Experimental verification of light induced field emission. <i>Applied Physics Letters</i> , 96(4), 044101. doi: 10.1063/1.3293297	This letter reports the experimental verification of the recently predicted phenomenon that the electric field emission current from a negatively charged surface gets enhanced by incidence of light (even of frequency below the photoelectric threshold) on the cathode.	cathodes; electric fields; field emission; photoelectricity				

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
Ghodake, G., Seo, Y. D., Park, D., & Lee, D. S. (2010). Phytotoxicity of carbon nanotubes assessed by Brassica juncea and Phaseolus mungo. <i>Journal of Nanoelectronics and Optoelectronics</i> , 5(2), 157-160. doi: 10.1166/jno.2010.1084	Two agronomic plant species were evaluated for the phytotoxicity of multi-walled carbon nanotubes (CNTs) using germination and seedling growth of Brassica juncea and Phaseolus mungo. Both B. juncea and P mungo seeds showed 100% germination with the application of CNTs, which indicated their non-hazardous nature for the germination of the seeds. As the B. juncea seed was grown with CNTs at 10 mu g/ml, 20 mu g/ml, and 40 mu g/ml, the enhancement of root growth was evidenced up to 138%, 202%, and 135%, respectively, compared to the control. In the case of B. juncea, the heights of the shoot and root were not affected at all by the studied CNTs' concentrations; however, phytotoxicity was evidenced at 40 mu g/ml CNTs by optical microscopy of the hairy root system, since a severe reduction in both the number of root hairs and their length was observed.	Phytotoxicity; Germination; Brassica juncea; Phaseolus mungo; Carbon nanotubes	bulk zno; toxicity; nanoparticles; behavior; tio2; nanomaterials; environment; spinach			
Hu, W., Zhang, X. B., Cheng, Y. L., Wu, Y. M., & Wang, L. M. (2011). Low-cost and facile one-pot synthesis of pure single-crystalline $\epsilon$ -Cu <sub>0.95</sub> V <sub>2</sub> O <sub>5</sub> nanoribbons: high capacity cathode material for rechargeable Li-ion batteries. <i>Chemical Communications</i> , 47(18), 5250-5252. doi: 10.1039/c1cc11184a	Pure single-crystalline epsilon-Cu <sub>0.95</sub> V <sub>2</sub> O <sub>5</sub> nanoribbons have been successfully synthesized via a facile one-pot solvothermal route using low-cost raw materials. The obtained materials can react electrochemically with 2.64 Li in a reversible fashion and thus greatly expands the range of cathode choices.		lithiation characteristics; electrochemical properties; electrode material; silicon nanowires; room-temperature; lithium; alpha-cu <sub>0.95</sub> v <sub>2</sub> o <sub>5</sub> ; gel			
Lai, S. L., Tan, W. L., & Yang, K. L. (2011). Detection of DNA targets hybridized to solid surfaces using optical images of liquid crystals. <i>ACS applied materials &amp; interfaces</i> , 3(9), 3389-3395. doi: 10.1021/am200571h	In this paper, we report a method of detecting DNA targets hybridized to a solid surface by using liquid crystals (LC). The detection principle is based on different interference colors of LC supported on surfaces decorated with single-stranded DNA (ssDNA) or double-stranded DNA (dsDNA). However, the contrast between the ssDNA and dsDNA is not obvious, unless DNA-streptavidin complexes are introduced to the dsDNA to increase the surface mass density. Two different approaches of introducing streptavidin to the system are studied and compared. We find that by premixing the biotin-labeled DNA targets with streptavidin prior to the DNA hybridization, branched-streptavidin complexes are formed and clear LC signal can be observed. This LC-based DNA detection principle represents an important step toward the development of a simple, instrument- and fluorophore-free DNA detection method.	liquid crystals; DNA microarray; DNA targets detection; single-stranded DNA; double-stranded DNA; Biotin; Streptavidin	gold surfaces; microarrays; amplification; transitions; technology; proteins; systems; arrays; probes			

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
<p>Wu, W. Q., Xu, Y. F., Rao, H. S., Su, C. Y., &amp; Kuang, D. B. (2013). A double layered TiO<sub>2</sub> photoanode consisting of hierarchical flowers and nanoparticles for high-efficiency dye-sensitized solar cells. <i>Nanoscale</i>, 5(10), 4362-4369. doi: 10.1039/c3nr00508a</p>	<p>We report the innovative development of a double layered photoanode made of hierarchical TiO<sub>2</sub> flowers (HTFs) as the overlayer and TiO<sub>2</sub> nanoparticles (TNPs) as the underlayer, for dye-sensitized solar cells (DSSCs). They were prepared via a mild and simple one-step hydrothermal reaction of TiO<sub>2</sub> nanoparticles/FTO glass substrate in an alkaline solution. The underlayer made of TNPs with a small size (20 nm in diameter) serves as a transparent photoanode for efficient dye adsorption. The overlayer consisting of HTFs (3-5 μm in diameter) embedded by TiO<sub>2</sub> nanosheets plays multiple roles in enhancing light-scattering and fast electron transport. DSSCs based on this novel double layered photoanode (5 μm TNPs + 5 μm HTFs) exhibit greater than 7.4% power conversion efficiency (PCE), which is higher than that of single layer TNP based photoanodes (6.59%) with similar thickness (similar to 10 μm), and this is mainly attributed to the superior light scattering ability and fast electron transport of the former. Meanwhile, the thickness of the TNP underlayer has been optimized to further improve the PCE and an excellent PCE of over 9% has been achieved based on a 15 μm TNP + a 5 μm HTF double layered photoanode, accompanied by a short-circuit photocurrent density of 17.85 mA cm<sup>-2</sup>, an open-circuit voltage of 763 mV and a fill factor of 0.67.</p>		<p>photovoltaic performance; conversion efficiency; nanowire arrays; morphology; spectroscopy; temperature; electrolyte; candidate; transport; spheres</p>			
<p>Wang, W. B., Li, X. H., Wen, L., Zhao, Y. F., Duan, H. H., Zhou, B. K., Shi, T. F., Zeng, X. S., Li, N., &amp; Wang, Y. Q. (2014). Optical simulations of P3HT/Si nanowire array hybrid solar cells. <i>Nanoscale research letters</i>, 9(1). doi: 10.1186/1556-276X-9-238</p>	<p>An optical simulation of poly(3-hexylthiophene) (P3HT)/Si nanowire array (NWA) hybrid solar cells was investigated to evaluate the optical design requirements of the system by using finite-difference time-domain (FDTD) method. Steady improvement of light absorption was obtained with increased P3HT coating shell thickness from 0 to 80 nm on Si NWA. Further increasing the thickness caused dramatic decrease of the light absorption. Combined with the analysis of ultimate photocurrents, an optimum geometric structure with a coating P3HT thickness of 80 nm was proposed. At this structure, the hybrid solar cells show the most efficient light absorption. The optimization of the geometric structure and further understanding of the optical characteristics may contribute to the development for the practical experiment of the promising hybrid solar cells.</p>	<p>P3HT; Si nanowire array; Hybrid solar cells; Finite-difference time-domain (FDTD) method</p>	<p>photovoltaic applications; absorption; enhancement; morphology; shell; layer; glass</p>			

Publications	Abstract	Keywords	Keywords_plus	Relevant	No relevant	Further comments
Hashimoto, K., Sasaki, F., Hotta, S., & Yanagi, H. (2016). Amplified Emission and Field-Effect Transistor Characteristics of One-Dimensionally Structured 2, 5-Bis(4-biphenyl) thiophene Crystals. <i>Journal of nanoscience and nanotechnology</i> , 16(4), 3200-3205. doi: 10.1166/jnn.2016.12285	One-dimensional (1D) structures of 2,5-bis(4-biphenyl)thiophene (BP1T) crystals are fabricated for light amplification and field-effect transistor (FET) measurements. A strip-shaped 1D structure (10 $\mu$ m width) made by photolithography of a vapor-deposited polycrystalline film shows amplified spontaneous emission and lasing oscillations under optical pumping. An FET fabricated with this 1D structure exhibits hole-conduction with a mobility of $\mu(h) = 8.0 \times 10^{-3}$ cm <sup>2</sup> /Vs. Another 1D-structured FET is fabricated with epitaxially grown needle-like crystals of BP1T. This needle-crystal FET exhibits higher mobility of $\mu(h) = 0.34$ cm <sup>2</sup> /Vs. This improved hole mobility is attributed to the single-crystal channel of epitaxial needles while the grain boundaries in the polycrystalline 1D-structure decrease the carrier transport.	One-Dimensional Structure; 5-Bis(4-biphenyl)thiophene; Amplified Spontaneous Emission; Organic Laser; Field-Effect Transistor	thiophene/phenylene co-oligomer; single-crystals			

### Appendix 9. Random sample with answers

Approach	Publication	No relevant	Relevant	No answer
A <sub>0</sub>	Lin, T., Zheng, K., Wang, C. L., & Ma, X. Y. (2007). Photoluminescence study of AlGaInP/GaN quantum well intermixing induced by zinc impurity diffusion. <i>Journal of Crystal Growth</i> , 309(2), 140-144. doi: 10.1016/j.jcrysgro.2007.09.029	55	42	1
A <sub>0</sub>	Ao, Y., Xu, J., & Fu, D. (2009). Study on the effect of different acids on the structure and photocatalytic activity of mesoporous titania. <i>Applied Surface Science</i> , 256(1), 239-245. doi: 10.1016/j.apsusc.2009.08.008	54	42	2
A <sub>0</sub>	Hu, W., Zhang, X. B., Cheng, Y. L., Wu, Y. M., & Wang, L. M. (2011). Low-cost and facile one-pot synthesis of pure single-crystalline $\epsilon$ -Cu <sub>0.95</sub> V <sub>2</sub> O <sub>5</sub> nanoribbons: high capacity cathode material for rechargeable Li-ion batteries. <i>Chemical Communications</i> , 47(18), 5250-5252. doi: 10.1039/c1cc11184a	16	81	1
A <sub>0</sub>	Ghalamestani, S. G., Heurlin, M., Wernersson, L. E., Lehmann, S., & Dick, K. A. (2012). Growth of InAs/InP core-shell nanowires with various pure crystal structures. <i>Nanotechnology</i> , 23(28), 285601. doi: 10.1088/0957-4484/23/28/285601	10	86	2
A <sub>0</sub>	Park, S., Lee, J., Do, I. G., Jang, J., Rho, K., Ahn, S., Maruja, L., Kim S. J., Kim, K. M., Mao, M., Oh, E., Kim, Y. J., Kim, J., & Choi, Y. L. (2014). Aberrant CDK4 amplification in refractory rhabdomyosarcoma as identified by genomic profiling. <i>Scientific reports</i> , 4, 3623. doi: 10.1038/srep03623	77	16	5
A <sub>1</sub>	Dechow, J., Forchel, A., Lanz, T., & Haase, A. (2000). Fabrication of NMR - Microsensors for nanoliter sample volumes. <i>Microelectronic engineering</i> , 53(1), 517-519.	62	32	4

Approach	Publication	No relevant	Relevant	No answer
A <sub>1</sub>	Hilleringmann, U., Vieregge, T., & Horstmann, J. T. (2000). A structure definition technique for 25 nm lines of silicon and related materials. <i>Microelectronic engineering</i> , 53(1-4), 569-572.	12	83	3
A <sub>1</sub>	Wilson, L. R., Carder, D. A., Steer, M. J., Cockburn, J. W., Hopkinson, M., Chia, C. K., ... & Airey, R. (2002). Strategies for reducing the emission wavelength of GaAs-AlAs quantum cascade lasers. <i>Physica E: Low-dimensional Systems and Nanostructures</i> , 13(2), 835-839.	51	43	4
A <sub>1</sub>	Du, X., & Hlady, V. (2002). Monolayer formation on silicon and mica surfaces rearranged from N-hexadecanoyl-L-alanine supramolecular structures. <i>The Journal of Physical Chemistry B</i> , 106(29), 7295-7299. doi: 10.1021/jp0209603	40	54	4
A <sub>1</sub>	Mao, C., Qi, J., & Belcher, A. M. (2003). Building Quantum Dots into Solids with Well-Defined Shapes. <i>Advanced Functional Materials</i> , 13(8), 648-656. doi: 10.1002/adfm.200304297	6	89	3
A <sub>1</sub>	Bao, M., Yang, H., Sun, Y., & French, P. J. (2003). Modified Reynolds' equation and analytical analysis of squeeze-film air damping of perforated structures. <i>Journal of Micromechanics and Microengineering</i> , 13(6), 795.	87	9	2
A <sub>1</sub>	Shi, Z., Wang, Q., Ye, W., Li, Y., & Yang, Y. (2006). Synthesis and characterization of mesoporous titanium pyrophosphate as lithium intercalation electrode materials. <i>Microporous and mesoporous materials</i> , 88(1), 232-237. doi: 10.1016/j.micromeso.2005.09.013	62	33	3
A <sub>1</sub>	Hájek, M., Veselý, J., & Cieslar, M. (2007). Precision of electrical resistivity measurements. <i>Materials Science and Engineering: A</i> , 462(1), 339-342. doi: 10.1016/j.msea.2006.01.175	85	12	1
A <sub>1</sub>	Bergman, L., Rosenholm, J., Öst, A. B., Duchanoy, A., Kankaanpää, P., Heino, J., & Lindén, M. (2008). On the complexity of electrostatic suspension stabilization of functionalized silica nanoparticles for biotargeting and imaging applications. <i>Journal of Nanomaterials</i> , 2008. doi: 10.1155/2008/712514	18	76	4
A <sub>1</sub>	Lai, S. L., Tan, W. L., & Yang, K. L. (2011). Detection of DNA targets hybridized to solid surfaces using optical images of liquid crystals. <i>ACS Applied Materials &amp; Interfaces</i> , 3(9), 3389-3395. doi: 10.1021/am200571h	54	39	5
A <sub>1</sub>	Yin, Z., Zheng, Q., Chen, S. C., Li, J., Cai, D., Ma, Y., & Wei, J. (2015). Solution-derived poly (ethylene glycol)-TiO <sub>x</sub> nanocomposite film as a universal cathode buffer layer for enhancing efficiency and stability of polymer solar cells. <i>Nano Research</i> , 8(2), 456-468. doi: 10.1007/s12274-014-0615-8	26	69	3
A <sub>1</sub>	Todai, M., Hagihara, K., Kishida, K., Inui, H., & Nakano, T. (2016). Microstructure and fracture toughness in boron added NbSi <sub>2</sub> (C40)/MoSi <sub>2</sub> (C11 b) duplex crystals. <i>Scripta Materialia</i> , 113, 236-240. doi: 10.1016/j.scriptamat.2015.11.004	76	18	4
A <sub>1</sub>	Gong, J., & Wilkinson, A. J. (2016). Sample size effects on grain boundary sliding. <i>Scripta Materialia</i> , 114, 17-20. doi: 10.1016/j.scriptamat.2015.11.029	75	21	2
A <sub>1</sub>	Hu, D., Wang, H. Y., & Zhu, Q. F. (2016). Design of an ultra-broadband and polarization-insensitive solar absorber using a circular-shaped ring resonator. <i>Journal</i>	68	28	2



Approach	Publication	No relevant	Relevant	No answer
	<i>of Nanophotonics</i> , 10(2). doi: 10.1117/1.JNP.10.026021			
A <sub>1</sub>	Hashimoto, K., Sasaki, F., Hotta, S., & Yanagi, H. (2016). Amplified Emission and Field-Effect Transistor Characteristics of One-Dimensionally Structured 2, 5-Bis (4-biphenyl) thiophene Crystals. <i>Journal of Nanoscience and Nanotechnology</i> , 16(4), 3200-3205. doi: 10.1166/jnn.2016.12285	38	52	8
A <sub>2</sub>	Alcala, M. D., Criado, J. M., Real, C., Grygar, T., Nejezchleba, M., Subrt, J., & Petrovsky, E. (2004). Synthesis of nanocrystalline magnetite by mechanical alloying of iron and hematite. <i>Journal of Materials Science</i> , 39(7), 2365-2370.	37	59	2
A <sub>2</sub>	Xiang, C., Yang, Y., & Penner, R. M. (2009). Cheating the diffraction limit: electrodeposited nanowires patterned by photolithography. <i>Chemical Communications</i> , (8), 859-873. doi: 10.1039/b815603d	5	92	1
A <sub>2</sub>	Sumesh, C. K., Patel, K. D., Pathak, V. M., & Srivastava, R. (2008). Twofold conduction mechanisms in molybdenum diselenide single crystals in the wide temperature range of 300K to 12K. <i>Chalcogenide Letters</i> , 5(8), 177-180.	79	17	2
A <sub>2</sub>	Borysenko, K. M., Mullen, J. T., Barry, E. A., Paul, S., Semenov, Y. G., Zavada, J. M., Nardelli, M. & Kim, K. W. (2010). First-principles analysis of electron-phonon interactions in graphene. <i>Physical Review B</i> , 81(12). doi 10.1103/PhysRevB.81.121412	32	64	2
A <sub>2</sub>	Vikram, S. V., Phase, D. M., & Chandel, V. S. (2010). High-TC phase transition in K2Ti6O13 lead-free ceramic synthesised using solid-state reaction. <i>Journal of Materials Science: Materials in Electronics</i> , 21(9), 902-905. doi: 10.1007/s10854-009-0015-0	83	12	3
A <sub>2</sub>	Ghodake, G., Seo, Y. D., Park, D., & Lee, D. S. (2010). Phytotoxicity of carbon nanotubes assessed by Brassica juncea and Phaseolus mungo. <i>Journal of Nanoelectronics and Optoelectronics</i> , 5(2), 157-160. doi: 10.1166/jno.2010.1084	30	66	2
A <sub>2</sub>	Westenfelder, B., Meyer, J. C., Biskupek, J., Kurasch, S., Scholz, F., Krill III, C. E., & Kaiser, U. (2011). Transformations of carbon adsorbates on graphene substrates under extreme heat. <i>Nano letters</i> , 11(12), 5123-5127. doi 10.1021/nl203224z	24	71	3
A <sub>2</sub>	Sherman, E. Y., Ban, Y., Gulyaev, L. V., & Khomitsky, D. V. (2012). Spin Tunneling and Manipulation in Nanostructures. <i>Journal of Nanoscience and Nanotechnology</i> , 12(9), 7535-7539. doi 10.1166/jnn.2012.6554	10	87	1
A <sub>2</sub>	Wu, W. Q., Xu, Y. F., Rao, H. S., Su, C. Y., & Kuang, D. B. (2013). A double layered TiO2 photoanode consisting of hierarchical flowers and nanoparticles for high-efficiency dye-sensitized solar cells. <i>Nanoscale</i> , 5(10), 4362-4369. doi: 10.1039/c3nr00508a	12	82	4
A <sub>2</sub>	Chiacchiarelli, L. M., Rallini, M., Monti, M., Puglia, D., Kenny, J. M., & Torre, L. (2013). The role of irreversible and reversible phenomena in the piezoresistive behavior of graphene epoxy nanocomposites applied to structural health monitoring. <i>Composites Science and Technology</i> , 80, 73-79. doi: 10.1016/j.compscitech.2013.03.009	34	58	6

Approach	Publication	No relevant	Relevant	No answer
A <sub>2</sub>	Foos, E. E., Yoon, W., Lumb, M. P., Tischler, J. G., & Townsend, T. K. (2013). Inorganic photovoltaic devices fabricated using nanocrystal spray deposition. <i>ACS applied materials &amp; interfaces</i> , 5(18), 8828-8832. doi: 10.1021/am402423f	22	74	2
A <sub>2</sub>	Wang, W. B., Li, X. H., Wen, L., Zhao, Y. F., Duan, H. H., Zhou, B. K., Shi, T. F. Zeng, X. S., Li, N., & Wang, Y. Q. (2014). Optical simulations of P3HT/Si nanowire array hybrid solar cells. <i>Nanoscale Research Letters</i> , 9(1). doi: 10.1186/1556-276X-9-238	18	74	6
A <sub>2</sub>	Shao Z. Q., Chen, J. W., Li Y. Q., & Pan, X.Y. (2014). Thermodynamical properties of a three-dimensional free electron gas confined in a one-dimensional harmonical potential. <i>Acta Physica Sinica</i> , 63(24). doi: 10.7498/aps.63.240502	79	17	2
A <sub>2</sub>	Soylemez, S., Udum, Y. A., Kesik, M., Hizliates, C. G., Ergun, Y., & Toppare, L. (2015). Electrochemical and optical properties of a conducting polymer and its use in a novel biosensor for the detection of cholesterol. <i>Sensors and Actuators B: Chemical</i> , 212, 425-433. doi 10.1016/j.snb.2015.02.045	69	27	2
A <sub>2</sub>	Dyshin, A. A., Eliseeva, O. V., Bondarenko, G. V., Kolker, A. M., & Kiselev, M. G. (2016). Dispersion of single-walled carbon nanotubes in dimethylacetamide and a dimethylacetamide–cholic acid mixture. <i>Russian Journal of Physical Chemistry A</i> , 90(12), 2434-2439. doi 10.1016/j.snb.2015.02.045	18	78	2
A <sub>3</sub>	Gotter, R., Ruocco, A., Butterfield, M. T., Iacobucci, S., Stefani, G., & Bartynski, R. A. (2003). Angle-resolved Auger-photoelectron coincidence spectroscopy (AR-APECS) of the Ge (100) surface. <i>Physical Review B</i> , 67(3), 033303. doi: 10.1103/PhysRevB.67.033303	78	16	4
A <sub>3</sub>	Nicolaidis, A. (2003). Singlet hydrocarbon carbenes with high barriers toward isomerization: A computational investigation. <i>Journal of the American Chemical Society</i> , 125(30), 9070-9073. doi: 10.1021/ja0299699	79	17	2
A <sub>3</sub>	Hichria, A., & Jazirib, S. (2003). Two Carriers in Vertically Coupled Quantum Dots: Magnetic Field Effect. <i>Journal of Nanoscience and Nanotechnology</i> , 3(3), 263-269. doi: 10.1166/jnn.2003.162	20	76	2
A <sub>3</sub>	Matsubara, M., Kortus, J., Parlebas, J. C., & Massobrio, C. (2006). Dynamical identification of a threshold instability in Si-doped heterofullerenes. <i>Physical Review Letters</i> , 96(15), 155502. doi: 10.1103/PhysRevLett.96.155502	43	51	4
A <sub>3</sub>	Chong, Y. M., Leung, K. M., Ma, K. L., Zhang, W. J., Bello, I., & Lee, S. T. (2006). Growing cubic boron nitride films at different temperatures. <i>Diamond and related materials</i> , 15(4), 1155-1160.	71	25	2
A <sub>3</sub>	Yang, P., Xu, R., Nanita, S. C., & Cooks, R. G. (2006). Thermal formation of homochiral serine clusters and implications for the origin of homochirality. <i>Journal of the American Chemical Society</i> , 128(51), 17074-17086. doi: 10.1021/ja064617d	64	31	3
A <sub>3</sub>	Stopa, M., & Marcus, C. M. (2008). Magnetic field control of exchange and noise immunity in double quantum dots. <i>Nano letters</i> , 8(6), 1778-1782. doi: 10.1021/nl801282t	20	77	1

Approach	Publication	No relevant	Relevant	No answer
A <sub>3</sub>	Gonzalez, J. (2008). Kohn-Luttinger superconductivity in graphene. <i>Physical Review B</i> , 78(20), 205431. doi: 10.1103/PhysRevB.78.205431	37	57	4
A <sub>3</sub>	Kanamadi, C. M., Das, B. K., Kim, C. W., Cha, H. G., Ji, E. S., Kang, D. I., Jadhav, A. P., & Kang, Y. S. (2009). Template assisted growth of cobalt ferrite nanowires. <i>Journal of Nanoscience and Nanotechnology</i> , 9(8), 4942-4947. doi: 10.1166/jnn.2009.1271	8	87	3
A <sub>3</sub>	Kher, S., Dixit, A., Rawat, D. N., & Sodha, M. S. (2010). Experimental verification of light induced field emission. <i>Applied Physics Letters</i> , 96(4), 044101. doi: 10.1063/1.3293297	78	16	4
A <sub>3</sub>	Bora, D. K., Braun, A., Erni, R., Fortunato, G., Graule, T., & Constable, E. C. (2011). Hydrothermal treatment of a hematite film leads to highly oriented faceted nanostructures with enhanced photocurrents. <i>Chemistry of Materials</i> , 23(8), 2051-2061. doi: 10.1021/cm102826n	25	72	1
A <sub>3</sub>	Fang, L., & Li, W. J. (2012). Hydrothermal synthesis of flake-like MnCO <sub>3</sub> film under high gravity field and their thermal conversion to hierarchical Mn <sub>3</sub> O <sub>4</sub> . <i>Micro &amp; Nano Letters</i> , 7(4), 353-356. doi: 10.1049/mnl.2011.0530	56	39	3
A <sub>3</sub>	Howell, S. L., Padalkar, S., Yoon, K., Li, Q., Koleske, D. D., Wierer, J. J., Wang, G. T., & Lauhon, L. J. (2013). Spatial mapping of efficiency of GaN/InGaN nanowire array solar cells using scanning photocurrent microscopy. <i>Nano Letters</i> , 13(11), 5123-5128.	9	88	1
A <sub>3</sub>	Gu, J., Xiao, P., Huang, Y., Zhang, J., & Chen, T. (2015). Controlled functionalization of carbon nanotubes as superhydrophobic material for adjustable oil/water separation. <i>Journal of Materials Chemistry A</i> , 3(8), 4124-4128. doi: 10.1039/c4ta07173e	15	80	3
A <sub>3</sub>	Meng, D., Wang, G., San, X., Shen, Y., Zhao, G., Zhang, Y., & Meng, F. (2015). CTAB-assisted hydrothermal synthesis of WO <sub>3</sub> hierarchical porous structures and investigation of their sensing properties. <i>Journal of Nanomaterials</i> , 16(1), 364. doi: 10.1155/2015/393205	30	64	4

## Appendix 10. Precision by experts' field and subfield of knowledge

### Precision by experts' field of knowledge

Approach	Biology	Chemistry	Computer science	Engineering	Materials science	Physics
A <sub>0</sub>	0,67	0,55	0,80	0,60	1,00	0,54
A <sub>1</sub>	0,60	0,45	0,73	0,66	0,62	0,45
A <sub>2</sub>	0,74	0,60	0,87	0,77	0,77	0,60
A <sub>3</sub>	0,72	0,49	0,87	0,72	0,79	0,57

### Precision by experts' nano subfield of knowledge

Approach	Nanobiomedicine	Nanobiosystems	Nanoelectronics	Nanoenergy	Nanoengineering	Nanofabrication	Nanomagnetism	Nanomaterials	Nanometrology	Nanooptoelectronics	Nanophotonics	Nanoprocesses	Nanoteoretical physics	Nanotoxicology & Sustainability
A <sub>0</sub>	0.72	0.58	0.51	0.60	0.64	0.76	0.50	0.55	0.40	0.75	0.39	0.60	0.50	0.67
A <sub>1</sub>	0.51	0.52	0.47	0.43	0.43	0.60	0.35	0.47	0.53	0.58	0.47	0.47	0.44	0.58
A <sub>2</sub>	0.71	0.72	0.59	0.57	0.67	0.67	0.55	0.58	0.73	0.57	0.60	0.64	0.57	0.73
A <sub>3</sub>	0.64	0.55	0.50	0.60	0.49	0.70	0.56	0.53	0.73	0.71	0.56	0.58	0.46	0.67

### Appendix 11. Differences between Step 5 and Step 7 of the approach at the journal level (A<sub>3</sub>)

#### Difference between Step 5 and Step 7

Step	NST data set	Number of journals	Number of excluded journal	Precision	Recall
5	WoS	123		0.89	0.75
7	Wos	110	31	0.89	0.67
5	Scopus	120		0.89	0.74
7	Scopus	108	34	0.90	0.65

### Precision and recall of the identified journals by the elbow criterion with threshold kink by figures

	Number of journals	Precision (p)	Recall
Figure 2	13	0.58	0.08
Figure 4	17	0.47	0.10
Figure 3	15	0.4	0.09
Figure 5	17	0.47	0.10

## Capítulo 11. Unveiling cognitive structure and comparative advantages of countries in knowledge domains

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### Abstract

Mapping and depicting the structure, dynamics and national specialization profiles of scientific fields at the country level affords a better understanding of national developments and changes in a given field, particularly when these changes may serve as an aid in decision-making with regard to research management. This paper looks at the cognitive structure of a field over time to characterize its development across countries and to appraise the competitiveness of countries in terms of research specialization. Based on a dataset extracted from the Scopus database, we conducted a co-word analysis and studied the degree of specialization based on publications and on keywords, in the Nanoscience and Nanotechnology field (NST). The results reveal that NST research tends to focus on nano applications and devices. According to the keyword activity index, the countries studied center their specialization on *electronic, biotechnology and biomedical research*, certain countries showing a more competitive edge in the global realm of output. Accordingly, implications that could contribute to decision-making regarding the economy and research policies are described.

### 1. Introduction

Characterizing scientific knowledge by tracking patterns, dynamics, and trends of scientific outcomes in a research field is useful for designing reliable and solid tools for science policy and science evaluation processes [1]. Through these patterns, the intellectual-cognitive structure and the dynamics of scientific fields over time can be explored [2] in order to provide an overview of emerging and/or mature research fields, and to perceive how

academic knowledge flows in the form of key concepts to be shared, recombined and developed over time [3].

However, depending on the level of aggregation, different approaches and units of analysis can be adopted. A combination of techniques (author co-citation analysis, document co-citation analysis, co-word analysis, etc.), units of analysis (journal, publication, keyword, etc.), and actors (countries, institutions, organizations, etc.) may lend accuracy to the identification and characterization of scientific fields [4,5].

Co-word analysis is considered an effective approach to investigate the knowledge structure and trends of domains. Co-word analysis can help describe, define and identify the research topics within a field. It gathers words from publications (usually extracted from titles, abstracts and keywords) to capture the changes in a field over time [6,7]. Through the study of terminology corresponding to different periods, co-word analysis draws a picture of cognitive structures and their development dynamics [8,9,10].

At the same time, characterizing national publications profiles serve to appraise countries' research strengths or weaknesses, which complement the analysis of the intellectual-cognitive structure. Based upon the idea that research topics of a particular field signal a country's specialization or diversification, hence its competitive advantages [11], relative indicators can be used to compare research performance in terms of the disciplinary specialization of countries.

The financing of research, development and innovation is based on variables such as relevance, excellence, innovation, quality, visibility, impact research and performance. To target the financing more effectively, evaluation and support of promising areas of research, innovation and technology is crucial. The idea is that countries can exploit their potential to become competitive if they take into account their strengths in terms of key activities within technological domains. Consequently, identifying domains and priority areas

while understanding stages of transition help improve competitiveness, knowledge growth and innovation capacity.

Nowadays, “Nanoscience and Nanotechnology” (henceforth NST) is an area holding vast technological and social potential for the community, presenting advancements for industry, health, the environment, and security. It therefore attracts great policy interest [12]. NST has been included as a promising strategic and innovative area in many research and development plans — even worldwide, e.g. the EU Research and Innovation Programme known as Horizon 2020 <sup>1</sup>, the National Science Foundation <sup>2</sup> and the National Nanotechnology Initiative<sup>3</sup>. Combining different approaches so as to grasp the global and local structure of the NST research field (here and thus far to test our proposal, a case study) should help trace its dynamics over time. This paper analyses cognitive structures and specialization profiles using the Activity Index, based on publications and on the use of keywords at global and country levels.

## **2. Literature Review**

Scientometric studies rely on diverse methods to explore the disciplinary structure, dynamics and research patterns of Nanoscience and Nanotechnology. Network analysis of WoS publications and subject categories were applied to establish the main scientific and technological fields (i.e. materials science, chemistry or physics) comprising NST research [13,14,15]. Citation analysis has previously been employed to identify the subject categories of NST publications from WoS [16], confirming that biomedical sciences were highly cited. Term analysis (extracted from titles, abstracts and keywords) of WoS publications have served to determine the main research topics of NST [17], to capture cutting-edge NST research [18], or to determine to what extent countries benefit from collaboration to heighten

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<sup>1</sup> [ec.europa.eu/programmes/horizon2020/en/what-horizon-2020](http://ec.europa.eu/programmes/horizon2020/en/what-horizon-2020)

<sup>2</sup> [www.nsf.gov](http://www.nsf.gov)

<sup>3</sup> [www.nano.gov](http://www.nano.gov)

research performance in terms of citation, leveraging competitiveness through the design of research and development agendas [19]. Hybrid methods — such as the combination of lexical mining, citation flows and mapping techniques— have been applied to nano publications from WoS to identify the diverse topics that comprise the NST field [20] or explore the dynamics of knowledge integration in some NST-related research areas [21].

Bibliometrics aid exploration of domains such as NST. Analyses of global NST scientific production based on WoS publications have revealed the main producers and contributors in NST output: China and South Korea underwent the most rapid growth in NST output, China being close to the overall leader —the US— and outstanding in certain nanotechnology research topics [22,23,24,25,26,27]. Similar outcomes were reported by Grieneisen and Zhang [28] and Arora et al. [16], who found that the top producers of NST publications were China, the US, Japan, Germany and South Korea, although a number of Asian (i.e. Taiwan, India or Iran) and European countries have become main contributors to the NST field [29]. Recent research found that Asia as a continent was the most productive in NST from 2000 to 2016, followed by Europe, whose main producers were Germany, the United Kingdom, France, Spain and Italy [30]. The most updated NST publication dataset shows China to lead in NST output, followed by the US; although European countries such as Germany and France make the top-ten worldwide ranking, respectively 4th and 8th [31].

The Specialization Index, a variation of the Activity Index (AI), is an indicator of whether a country has a relatively high or low share in world publications within a particular field or domain. The AI per se has been employed to study the disciplinary evolution of some countries [32,33,34,35], while versions of the AI include the revealed comparative advance [36], the Attractivity Index [37], Document-Type variant [38] or Keyword Activity Index [39], and similarity measures applied to scientific collaboration [40]. For a comprehensive review of this indicator, we would refer to Rousseau [41].



Based on this idea, the use of the Keyword Activity Index would identify the most representative keywords in a more effective way because it also considers low-frequency keywords. These pertain to emergent and innovative concepts of a domain, and may distinguish the most dynamic areas in sub-domains [42].

Not many bibliometric analyses of global NST scientific production have been based on Scopus publications, despite its vast coverage [43,44]. Although the main players and contributors in NST have been explored, to date the national country profile in terms of specialization in NST has hardly been studied [45]. To support an efficient distribution of funds, however, a deeper exploration of promising areas at the national or even at the European Union level might prove essential.

### **3. Objectives**

The aims of this paper are to (1) proceed with a characterization of NST by means of a reliable and detailed search strategy, (2) discern the evolution over time of the cognitive structure of a given scientific discipline, and (3) trace its specialization profile from a twofold perspective: publications plus keywords. Accordingly, this study updates previous outcomes [17,46,47] by extending the time period studied, and refining the search strategy [12]. Our approach should help arrive at a better understanding of a field's development and comparative advantages at the country level. To test it, we used the Scopus database to fill in gaps of previous studies that relied on WoS research topics in addressing specific research questions:

RQ1: Worldwide, which countries are the main producers, how has their output evolved, and what comparative degree of specialization have they achieved?

RQ2: What are the main research topics in NST at the worldwide level, and how do European countries —Germany, France and Spain— perform in terms of their cognitive contributions to the development of NST research topics?

RQ3: Considering the use of keywords, how specialized are countries in each research topic? How do they reflect the scientific profile of NST and its evolution over time?

#### **4. Data and method**

Data were retrieved from Scopus database at the global and country level using an updated and refined search strategy (Supplementary Text S1) described in Muñoz-Écija et al. [12]. Following Wang et al. [31], we focus our analysis at the country level on Germany, France and Spain as the main European producers in NST, given that the United Kingdom left the European Union in 2020. We aim to see how Spain's NST output performs in comparison with that of other European countries. This focus was adopted with the understanding that the European Union is strategically committed to the development of nanotechnology in the framework of a global knowledge-based economy. Indeed, the EU funds projects undertaken by its member states overall, while encouraging nanotechnology research endeavors.

Previous studies look into the NST cognitive structure [17] and specialization [45] until 2013. So as to broaden the scope of these previous studies, past decade's first year (2010), middle year (2014), and final year showing complete data for bibliometric analysis (2018) were analyzed. That is, to visualize the cognitive structure of NST and its evolution, a temporal division was made into three different years, with a 4-year gap between them. Data at the global level were used to build overlay maps serving as reference for the analysis of several countries. A single representation for the full period (2010-2018) would not allow us to appraise evolution and would imply a loss of information, showing consolidated fields but not detecting emerging fields or the interactions among diverse research fronts. For this reason, we focused

on those three years as representative of a total duration of nine years (2010, 2014 and 2018), in order to perceive changes over time in the NST research field. The NST dataset comprises 396,250 publications, including all document types (Supplementary Information. Table S1).

#### **4.1. Co-word maps**

Co-word analysis (Callon et al., 1991) has been outlined and later substantiated (Leydesdorff & Nerghe, 2017) as the best method to identify the cognitive structure of a field at the level of research specialties. Furthermore, it is capable of revealing new developments within a research topic over time (Vargas-Quesada et al., 2017). To perform co-word analysis, we used the keywords (author keywords and indexed keywords) contained in all the retrieved documents to build a proximity/similarity matrix. A threshold of co-occurrence  $\geq 10$  was set to generate the cognitive structure. In order to avoid synonymy and acronymy issues, we normalized the keywords by designing an *ad hoc* thesaurus (Supplementary Text S2), standardizing plural and singular, abbreviation or acronyms, as complete keywords.

Science mapping —to intuitively analyze co-word maps— consists of developing and applying computational techniques for the visualization, analysis and modeling of a wide range of scientific and technological activities (Chen et al., 2015a); it is intended to display structural and dynamic aspects of scientific research (Börner et al. 2005; Moya-Anegón et al., 2007; Alcaide-Muñoz et al., 2017). Local science maps are problematic when it comes to comparisons because their units or positions of representation are not stable. To overcome this, one can take the units and the positions derived from a global map of science, then superimpose upon them the information to be displayed and analyzed (Rafols et al., 2010). Such “overlay maps” are a powerful tool, serving to explore an activity of interest (e.g. publications of a given organization, the references used in an emergent field, co-words...) and appraise the increasingly fluid and complex dynamics of the sciences (Rafols et al., 2010; Leydesdorff et al., 2013; Carley et al., 2017; Vargas-Quesada et

al., 2017). NST co-word maps at the global level in 2010, 2014 and 2018 were constructed, and the corresponding overlay maps for each year were derived for Germany, France and Spain, in order to explore and compare cognitive structures and main research topics.

Mapping was performed using VOSviewer (van Eck & Waltman, 2010). Each node/circle represents a keyword. The circle's size reflects the number of times it occurs in the document represented. The level of co-occurrence (how frequently keywords co-occur) is expressed by the distance between two keywords —that is, the closer two keywords are, the stronger their relationship is. The colors represent the different clusters (research topics) detected. Then, the keywords of high frequency were extracted as the basis for our analysis, since keywords of this nature usually coincide with research hotspots.

#### **4.2. Activity index**

The Activity Index (AI) or Specialization Index, introduced by Frame [32], is a version of the Revealed Comparative Advantage Index (RCA) used more commonly in Economics to quantify the economic/production advantages of countries [55]. In this study, the AI denotes the relative research effort that a country devotes to a given subject field, i.e. the publication profile of national research in a given country, by measuring whether “a country has a relatively higher or lower share in world publications in a particular field of science than its overall share in world total publications” [56], and is defined as:

$$AI = \frac{\text{the share of the given field in the publication of the given country}}{\text{the share of the given field in the world total of publications}}$$

When AI is greater than one, it means that the country's research production in a given field is higher than the world average, just as  $AI \leq 1$  means lower

than the world average. In order to assess each country's relative disciplinary strengths in NST, we apply the Relative Specialization Index (RSI). Thus,  $RSI \geq 0$  versus  $\leq 0$  indicates scientific specialization or no specialization of a country in a given field. RSI is defined as:

$$RSI = \frac{AI - 1}{AI + 1}$$

Hence, we calculated the AI and RSI in 2010, 2014 and 2018 to estimate their NST publication profile over time and detect changes in specialization or comparative advantages [34].

Following this framework, to estimate the comparative advantages of a country in a given research topic, the notion behind the Activity Index for publications is applied to the keywords. Because the AI designates whether a certain country has comparative advantages in researching a certain topic, it facilitates the selection of country-specific topics [57]. The Activity Index variant based on keywords (KAI) is defined as:

$$KAI = \frac{\text{the share of a given research topic in the keyword of a given country}}{\text{the share of a given research topic in the world total keywords}}$$

$KAI \geq 1$  indicates that a topic is emphasized in the country above its average level, and  $KAI \leq 1$  that the topic is underemphasized in that particular country. In order to assess each country's relative disciplinary strengths based on keywords, we apply the Relative Specialization Index (RSIk). Accordingly,  $RSIk \geq 0$  versus  $\leq 0$  indicates scientific specialization or no specialization of a country in a given field. RSIk is defined as:

$$RSIk = \frac{KAI - 1}{KAI + 1}$$

Sometimes high-frequency keywords from publications denote general concepts used by many researchers of a given field, without accurately

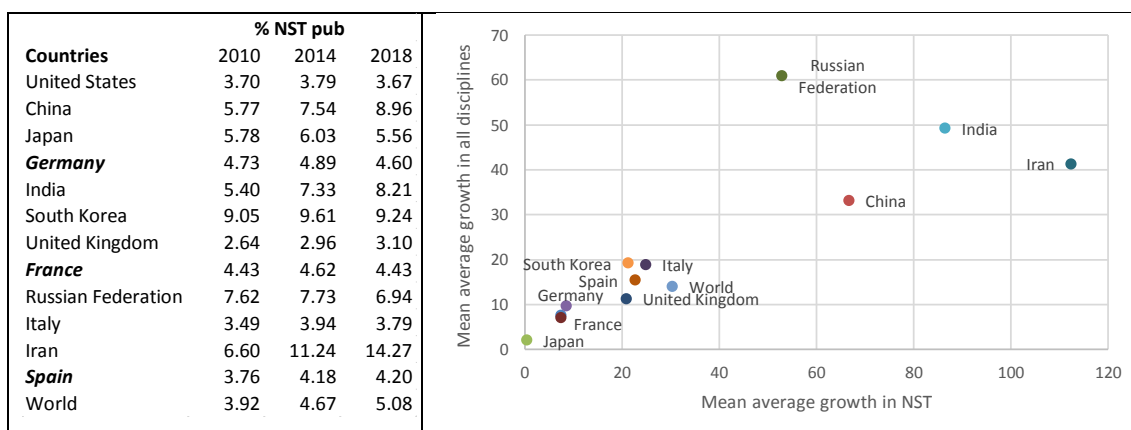
representing details of a field, especially regarding topics that may be the strength of a single country [39]. In turn, low-frequency keywords reflect innovative and emerging concepts, being more representative than their high-frequency counterparts [42]. The present article puts forth a means of identifying keywords in view of the frequency of their use in the world and in certain countries. The science maps that display the entire NST keywords clearly show the most relevant keywords in one or more countries. Being lesser than the number of total keywords, these specific keywords act as spotlights that more clearly expose the research advantages of countries under bibliometric study.

## 5. Results

### 5.1. Basic statistics

Bearing in mind the countries producing more than 50,000 documents in the period 2010-2018, among them the countries studied here, Figure 1 shows the percentage of NST documents published with respect to total output in each country and worldwide for the years 2010, 2014 and 2018 (left). The United States and China are the outstanding NST producers (22,534 and 19,883 documents, respectively), followed by Japan and Germany (7,534 and 7,322) (see Supplementary Information. Table S1).

**Figure 1.** Percentage of NST publications at the global and country level in 2010, 2014 and 2018 (left) and mean average growth rate in NST and in all disciplines (right)

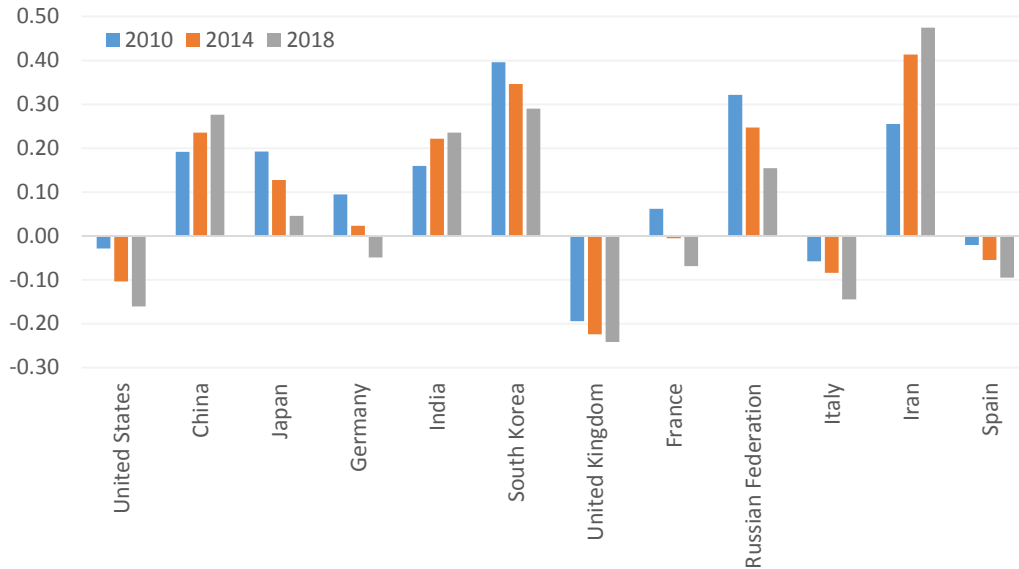


The graph on the left shows, for the same geographic aggregates, the average rate of growth for the entire period. At the global level, the share of world output reflects a steady increase in NST publications: a 30% annual growth rate over the nine years analyzed (Figure 1-right). At the country level, even though the raw number of publications increases year by year, growth is not homogenous —Iran, India, China and the Russian Federation increase their output much more than the rest of the world, or the other main producers, and well above the level of output in all other disciplines (Supplementary Information. Table S2). These results largely agree with previous reports of how countries follow different dynamics and output processes in NST [45]. Among the three countries targeted in this study, Germany shows the highest proportion of NST output, followed by France, while Spain presents the highest annual growth rate.

## **5.2. Relative Specialization Index based on publications**

Figure 2 presents the relative specialization index of the most prolific countries in NST considering their production in this field in comparison with the total production in all disciplines and taking the world as a standard (0).

In Germany, France and Spain, the corresponding RSI value is seen to decline after 2010. It may be that these countries are more specialized in nano applied research than in nano basic research. Similar results were divulged by Porter et al. [18], with Germany and France showing a decrease in the NST cutting-edge research activity (2006-2015), perhaps due to a growing interest in nano applications, for instance those related to biomedical research. This also means that other countries are increasing their specialization in the NST field. Indeed, Iran, India and South Korea show substantial specialization growth after 2010 (Supplementary Information. Table S3).



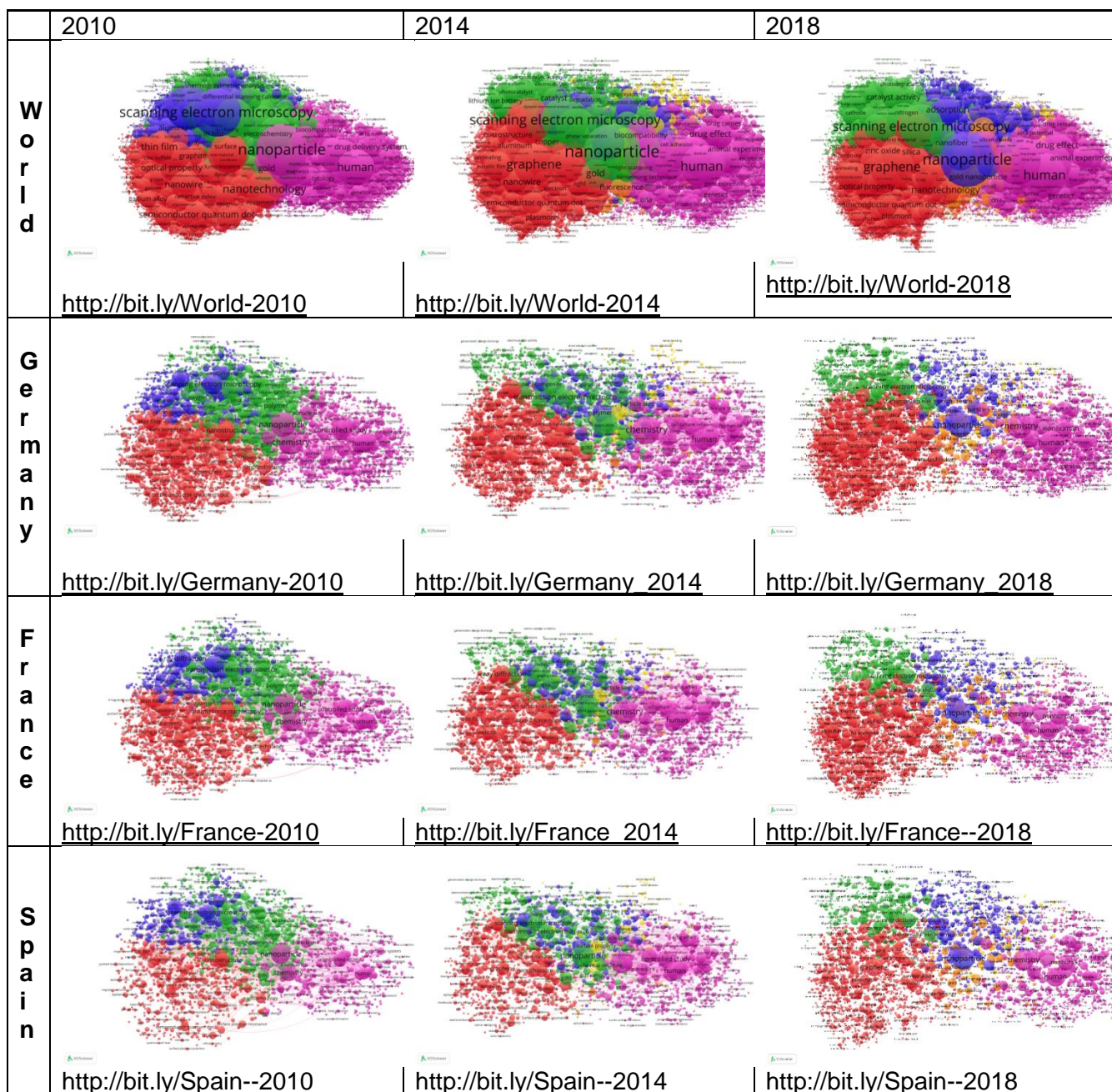
**Figure 2.** Relative Specialization Index in NST for the most prolific countries in the period 2010-2018

### 5.3. Co-word maps

Figure 3 displays the knowledge structure of NST over time using science overlay maps. At the worldwide level, the networks represent structures having different numbers of research topics and a variety of keywords in each line. All research topics identified in the world over time are transferred and represented at the country level. The number of keywords defines the disciplinary matrix calculated by co-occurrence that determines one's position in the hierarchy. The 50 most frequent keywords occurring for the world, for Germany, France and Spain—in descending order of prevalence by their occurrence and the total number of overlapped keywords per research topic—can be consulted in the Supplementary Information, Data S1, S2 and S3.

In these global maps, the hierarchical clustering reveals a structure with four research topics in 2010: *Microelectronics engineering and top-down processes* (red), *Synthesis of nanomaterials and bottom-up processes + Optics and electronics* (green), *Biotechnology and Biomedicine* (purple), and *Physical and mechanical characteristics of materials* (blue). However, the research topic *Biotechnology and Biomedicine* becomes divided into three





**Figure 3.** Global co-word maps for each country and the world output in NST.

The links at the bottom of each map allow the reader to visualize and zoom in the maps and the networks on VOSviewer, for example, from the 2,117 nodes of the Spanish domain and its 991,186 links in 2010, to the 6,588 nodes of Germany in 2018, with their corresponding 3,515,751 links. Please note that for very broad domains, e.g., the world map, a computer with more than 16 GB of RAM is needed to see the maps clearly.

new clusters in 2014, lasting until 2018. These emergent clusters are still related with *Biotechnology and Biomedicine*, but they show greater

specialization, in: 1) therapeutic applications through the distribution of medicines; 2) diagnostic techniques using biosensors; and 3) regenerative medicine. Thus, the specialization of the research topic *Biotechnology and Biomedicine* gives rise to the following clusters: *Biotechnology and Biomedicine: Therapeutic biomedicine* (purple); *Biotechnology and Biomedicine: Regenerative medicine* (light yellow); and *Biotechnology and Biomedicine: Biosensing* (orange).

As the global co-word maps show, the development of NST has meant the emergence of new research topics related with the application of NST for the purposes of social well-being, as in the biomedical field (clusters colored in purple, orange and light yellow). The research topics of NST based on physics, chemistry, and materials science, whether theoretical or conceptual, are represented by research topics colored in red, green and blue. These three research topics are essential for manufacturing procedures involved in the development of new materials, as well as technological devices.

Over the years, NST research appears to have remained stable in Physics and Chemistry (clusters colored in green and in blue), key domains for its evolution. But noteworthy interest in the biomedical applications (clusters in purple, orange and light yellow) results in a greater specialization of researchers along new research topics. In this sense, NST research related to new materials and engineering fields (colored in red) has increased gradually every year, but less than in the area of biomedical research.

At the country level, Germany focuses on *Microelectronics engineering and top-down processes* (red) and *Biotechnology and Biomedicine* (purple) research, and undergoes minor growth in research based on *Physical and mechanical characteristics of materials* (blue). France shows a pattern similar to Germany's at first; but its trend in NST research changed in 2014 and 2018, with a remarkable increase in *Biotechnology and Biomedicine*. This development gave rise to new research topics in the biomedical and

biotechnological field or increased the existing research in the case of *Therapeutic biomedicine*. Spain largely follows the behavior of Germany or France in that *Microelectronics engineering and top-down processes* (red) became the top research topic after 2010. Yet unlike the others, *Synthesis of nanomaterials and bottom-up processes + Optics and electronics* (green) decreased in terms of the number of overlapped keywords after 2014.

Worldwide, the top keywords used in each research topic show only slight differences by year. At the worldwide level, nanoparticle is the keyword that tops the ranking every year along with *scanning electron microscopy* and *chemistry*. There are some differences among the remaining top-five keywords, however. For example, *x ray diffraction* appears only in 2010 and 2014. Human was a top keyword in 2014, and again in 2018. *Graphene* appears as a top keyword only in 2018. At the country level, the keywords *nanoparticle*, *graphene*, *human* and *chemistry* showed the highest overlap with the world maps for Germany. In France, the most overlapped keywords were *nanoparticle*, *human*, *controlled study* and *unclassified drug*. For Spain, *nanoparticle*, *chemistry* and *graphene* were the outstanding keywords.

#### **5.4. Relative Specialization Index based on keywords in each research topic**

Table 1 shows the RSIk from a dual perspective. For one, the average RSIk of each cluster is calculated in terms of the total number of keywords (N terms). Secondly, the average RSIk is calculated in terms of the total occurrences (N occurrences). As can be seen in Figure 1, Germany, France and Spain show a specialization under 0 with respect to world output and to that of other countries. Because this value is lower than 0, we find specialization with values under 0 when we look at the terms of the different research topics comprising NST in the countries studied (Table 1). But if we look at specialization when calculated based on total term occurrences, most values are over 0 with respect to the world. That is, after eliminating the size

effect from output, we discover which countries have a research topic with a competitive edge on the global level.

This cross-country comparison regarding patterns of specialization evidences noteworthy differences. The RSIk values (total number of terms) reveal that in Spain, all the NST research topics have relative advantages between 2010 and 2018, though *Biotechnology and Biomedicine: Therapeutic biomedicine* reflects the greatest advantage. France shows a relative advantage in *Microelectronics engineering and top-down processes* research, whereas Germany evolves toward specialization in *Biotechnology and Biomedicine: Therapeutic biomedicine*, as does Spain, but to a lesser extent (Table 1).

In turn, the RSIk values (total number of occurrences) (Table 1) present greater advantages in all the research topics in Spain at the worldwide level in the period 2010-2018, especially in the areas of *Biotechnology and Biomedicine* and the characterization of nanomaterials. The lowest advantages are seen for Germany, giving values of 0 in *Physical and mechanical characteristics of materials*, or under 0 as is the case of *Synthesis of nanomaterials and bottom-up processes + Optics and electronics*. France shows intermediate values, between Germany and Spain, in all the research topics, although it has a greater advantage in research related with engineering.

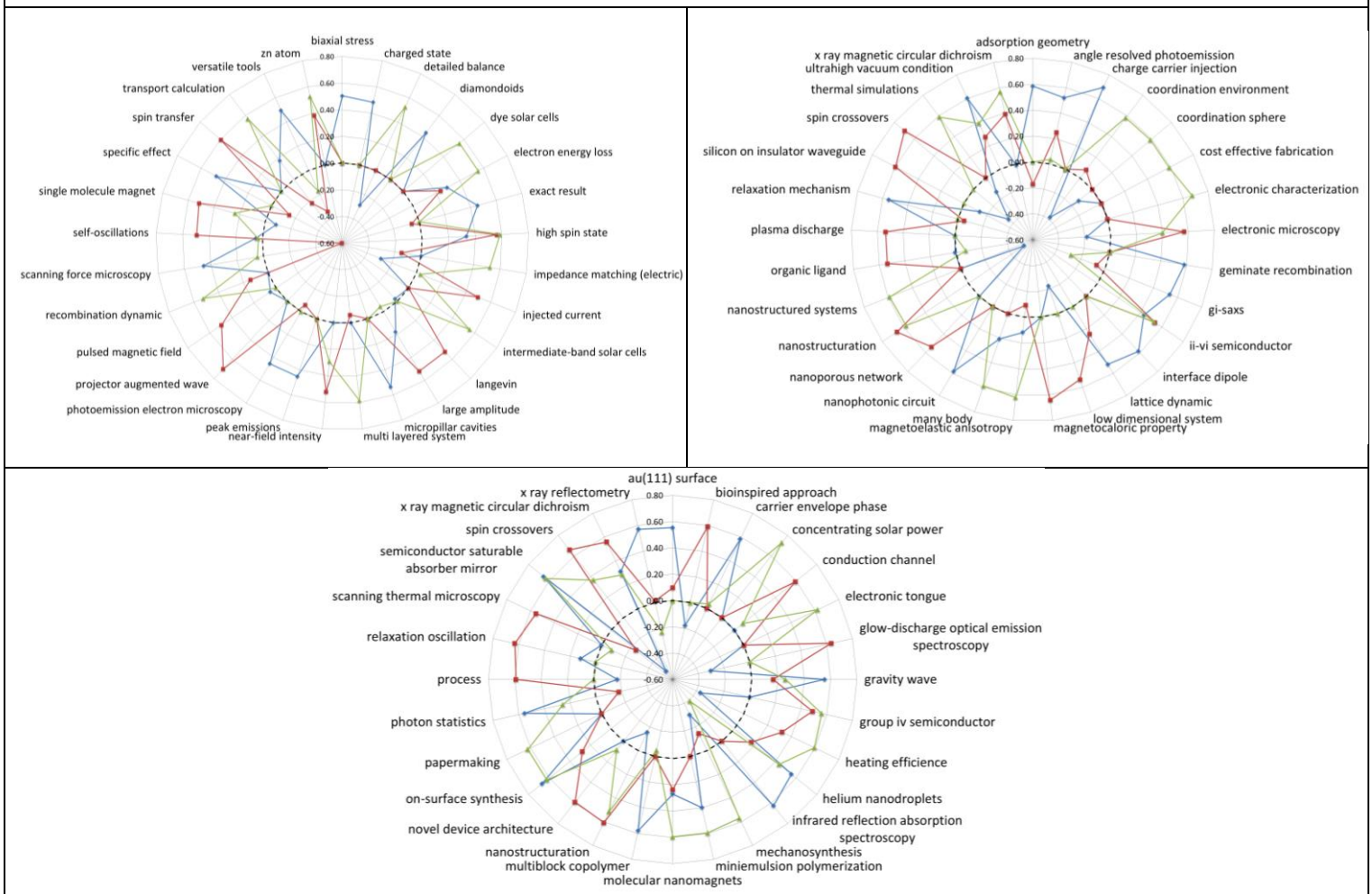
Figure 4 indicates the top 10 RSIk of each research topic. Each cluster is described below for more detailed analysis. Further details can be found in the Supplementary Information, Data S1, S2 and S3.

**Table 1.** RSI of each research topic based on keywords

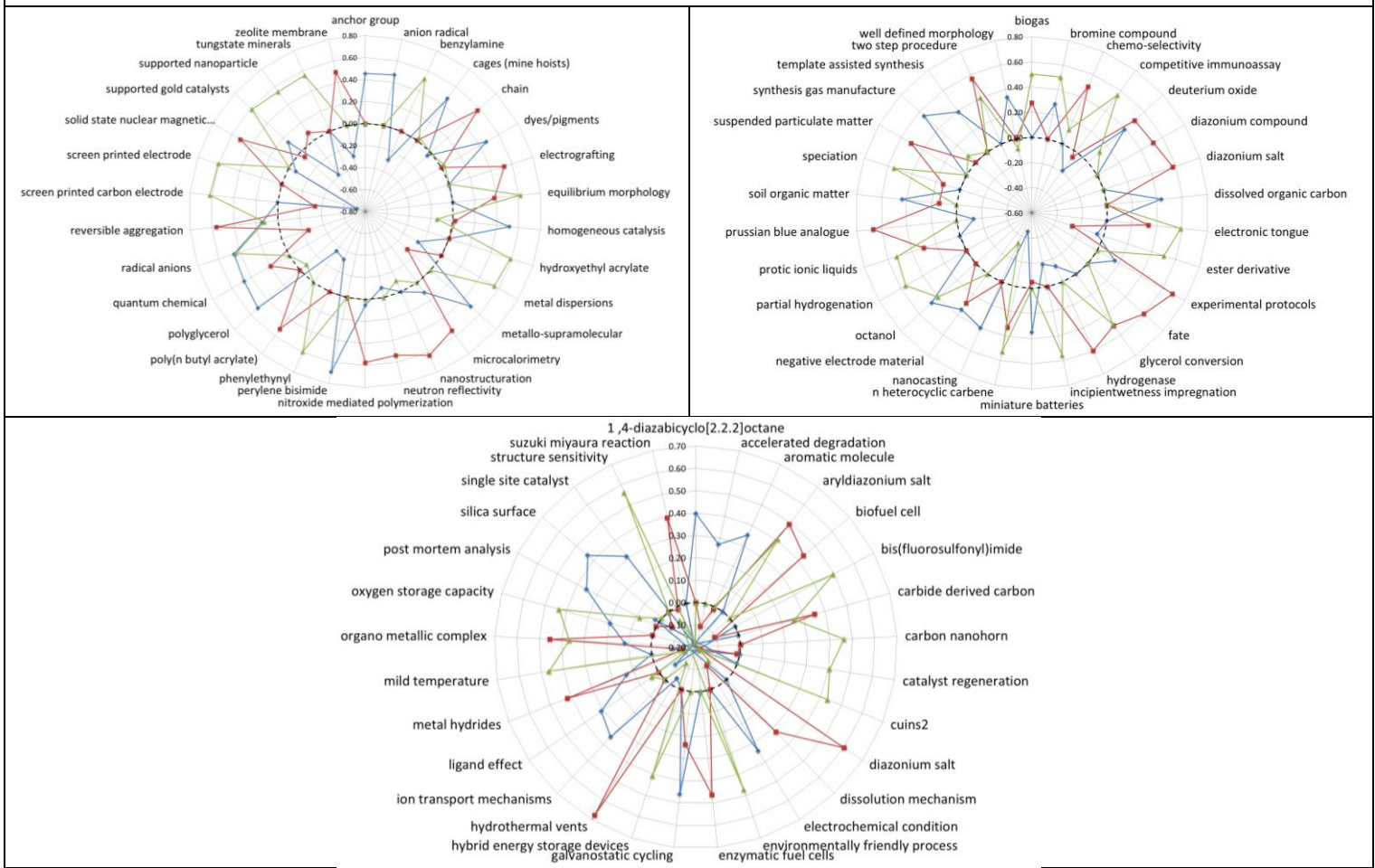
		Microelectronics engineering and top-down processes			Biotechnology and Biomedicine: Therapeutic biomedicine			Synthesis of nanomaterials and bottom-up processes + Optics and electronics			Physical and mechanical characteristics of materials			Biotechnology and Biomedicine: Regenerative medicine			Biotechnology and Biomedicine: Biosensors		
		G	F	S	G	F	S	G	F	S	G	F	S	G	F	S	G	F	S
2010	N terms	-0.35	-0.33	-0.32	-0.34	-0.37	-0.32	-0.36	-0.36	-0.26	-0.41	-0.38	-0.31	--	--	--	--	--	--
	N occurrences	0.12	0.20	0.23	0.13	0.16	0.24	0.11	0.17	0.30	0.05	0.15	0.25	--	--	--	--	--	--
2014	N terms	-0.30	-0.30	-0.30	-0.29	-0.30	-0.25	-0.41	-0.36	-0.29	-0.35	-0.31	-0.25	-0.40	-0.44	-0.27	-0.39	-0.39	-0.31
	N occurrences	0.13	0.19	0.20	0.15	0.19	0.26	0.01	0.11	0.20	0.09	0.17	0.25	0.17	0.13	0.27	0.03	0.09	0.19
2018	N terms	-0.30	-0.28	-0.31	-0.29	-0.32	-0.27	-0.47	-0.44	-0.37	-0.43	-0.39	-0.28	-0.44	-0.50	-0.38	-0.36	-0.37	-0.30
	N occurrences	0.15	0.23	0.20	0.17	0.19	0.25	-0.05	0.04	0.12	0.00	0.10	0.24	0.05	0.05	0.25	0.08	0.12	0.22

G=Germany; F=France; S=Spain. \*Cell color scale red-white-blue. Red color is assigned to the lowest value, and blue color to the highest value. Other values are assigned a weighted blend of colors.

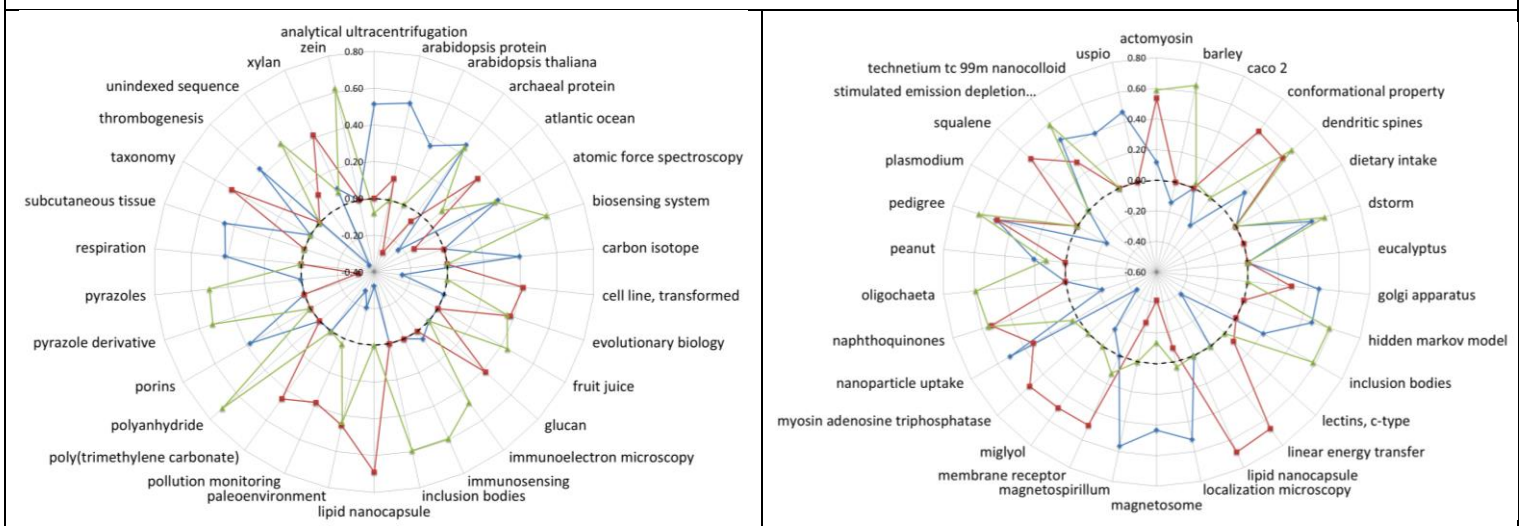
**Red cluster: Microelectronics engineering and top-down processes**

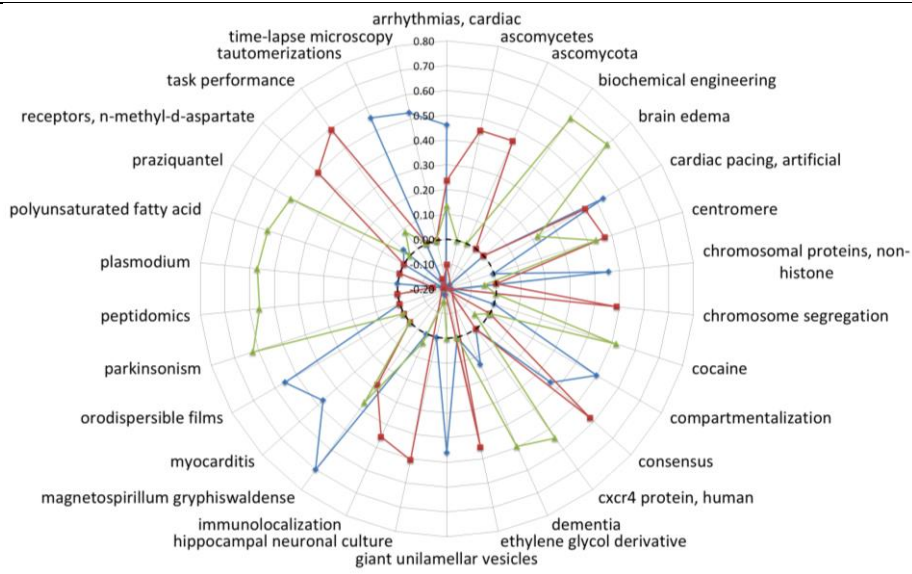


## Green cluster: Synthesis of nanomaterials and bottom-up processes + Optics and electronics

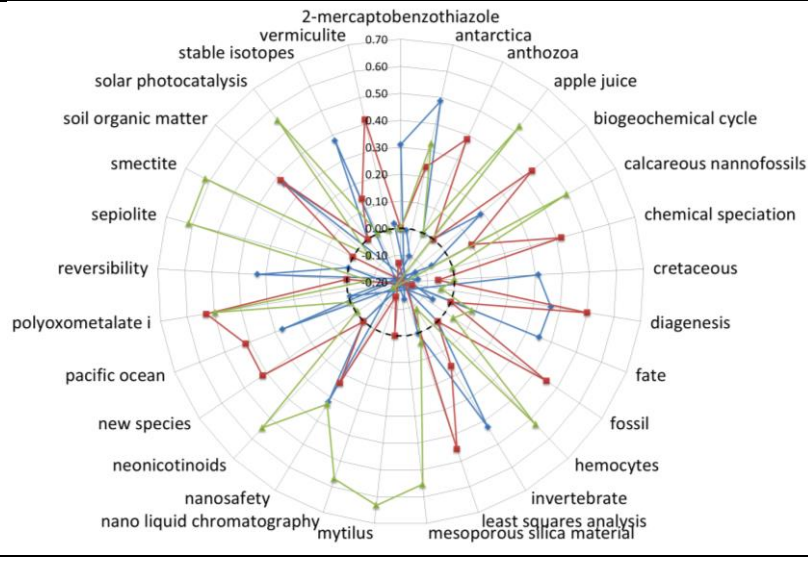
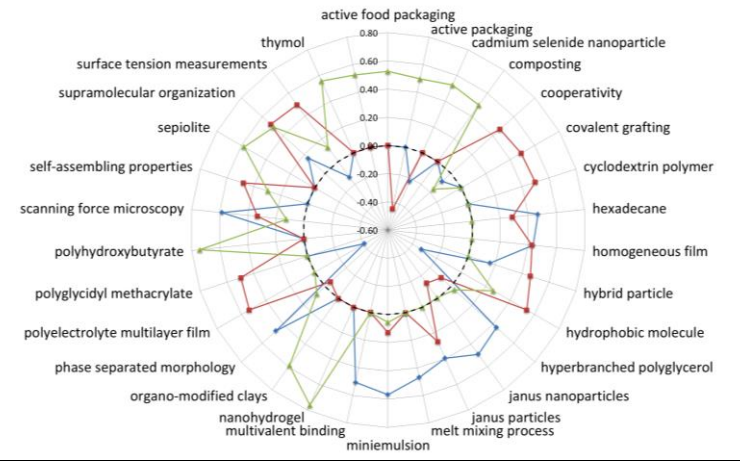
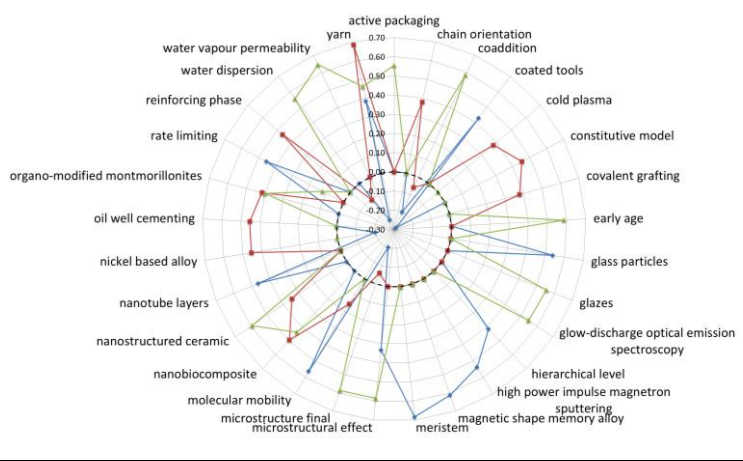


## Purple cluster: Biotechnology and Biomedicine - Therapeutic biomedicine



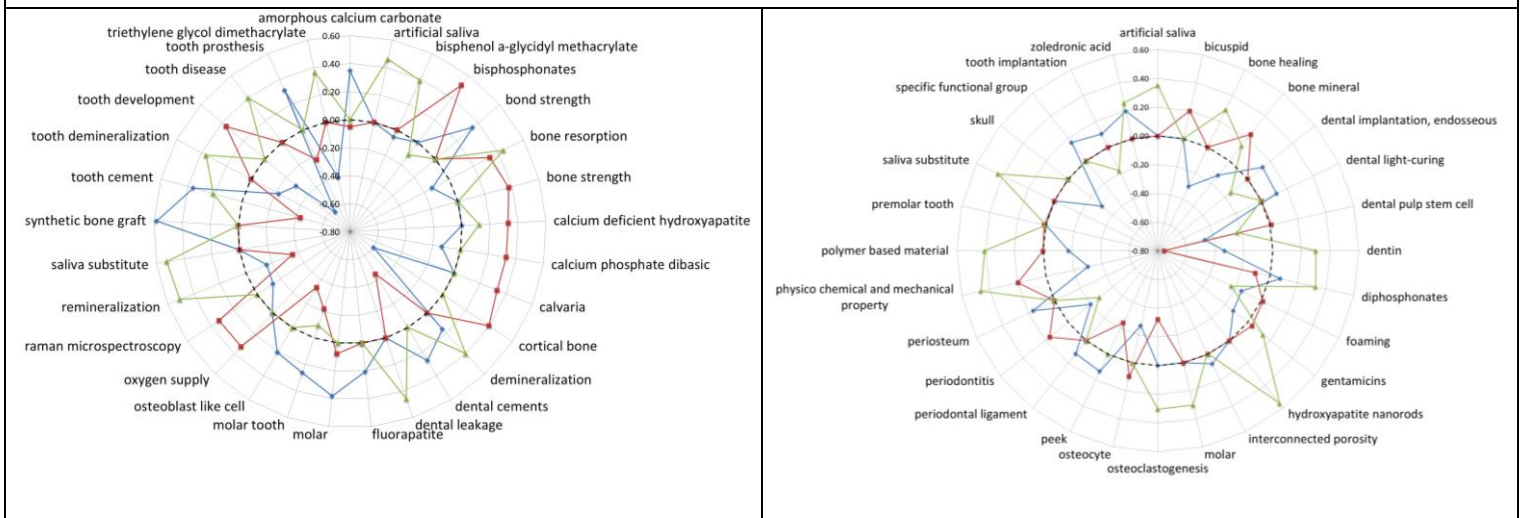


Blue cluster: Physical and mechanical characteristics of materials



Light yellow cluster: Biotechnology and Biomedicine - Regenerative medicine

Research topic is not detected in 2010.



Orange cluster: Biotechnology and Biomedicine - Biosensing

Research topic is not detected in 2010.

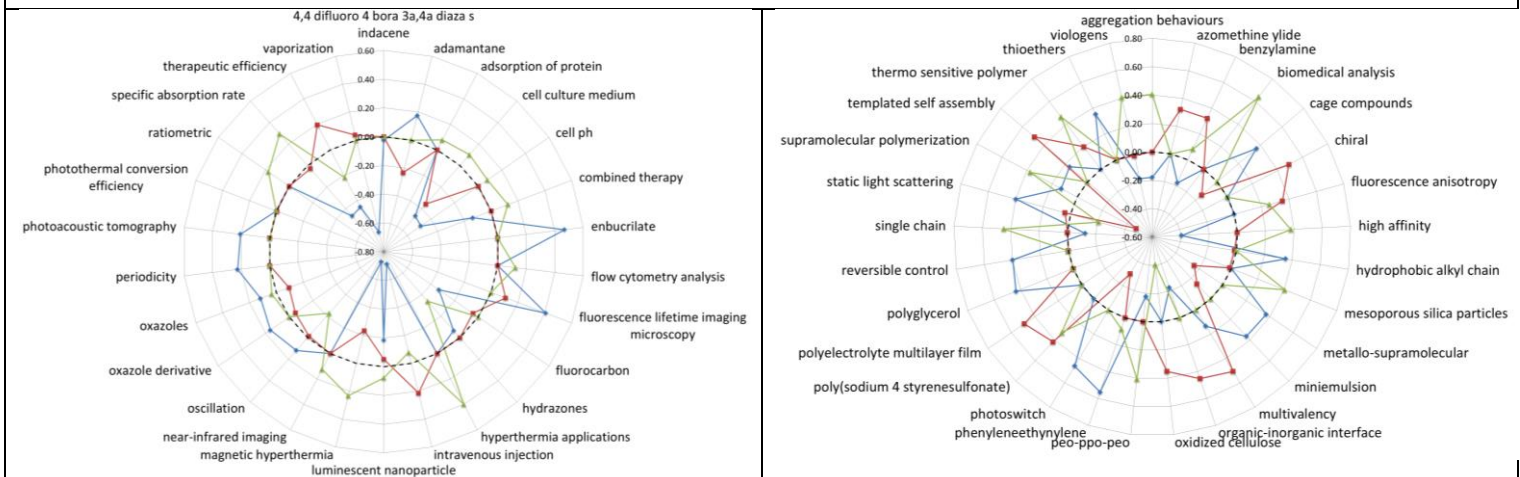


Figure 4. Top 10 RSIk keywords in each cluster in Germany (blue), France (red) and Spain (green)

5.4.1. Microelectronics engineering and top-down processes – red cluster

In 2010, this research topic has a relative advantage in *micropillar cavities* and *biaxial stress* in Germany. In France, this advantage is highest in terms that include *projector augmented wave*, *spin transfer* or *high spin state*. The latter term, *high spin state*, coincides with one of the keywords denoting



higher specialization in Spain, along with other terms, such as *dye solar cells*, that reflect intensive activity.

In 2014, the term *carrier injection* presents the highest relative advantage in Germany. The terms relative to spin, e.g. *spin crossovers*, continue to indicate high research activity in France, although other terms arise, among them *nanostructuring* or *x ray magnetic circular dichroism*. In Spain, new terms related with major advantages include *nanostructured systems*, as well as *nanostructuring* or *x ray magnetic circular dichrois*, keywords coinciding with those of France.

In 2018, a new term signaling relative advantages is *semiconductor saturable absorber mirror*. In Francia, *spin crossovers* and *nanostructuring* continue to denote high relative advantages; and *x ray magnetic circular dichroism* shows remarkable growth when compared with 2014. Researchers in Spain funneled more effort into *concentrating solar power* and *semiconductor saturable absorber mirror*; and whereas *nanostructuring* and *x ray magnetic circular dichroism* continued to mark research activity, it was less than in 2014.

#### **5.4.2. Synthesis of nanomaterials and bottom-up processes and Optics and electronics – green cluster**

In 2010, Germany reveals major research activity in *perylene bisimide*, *homogeneous catalysis* and *polyglycerol*, whereas France initially concentrates more research specialization on *nanostructuring* or *nitroxide mediated polymerization*. In Spain, the term highlighting research advantages is *screen-printed carbon electrode*.

In 2014, new terms appear: for example, *synthesis gas manufacture* or *octanol* in Germany. The research activity in France is more heavily dedicated to *experimental protocols* or *prussian blue analogue*. In Spain the terms vary, with the emergence of terms such as *electronic tongue* or *competitive immunoassay*.

In 2018, greater research activity is focused on terms such as *galvanostatic cycling* and *silica surface* in Germany. In France, *diazomiun salt* rises as a relative advantage keyword, and new terms such as *hydrothermal vents* or *aryldiazonium salt* mark the bulk of research activity. Spain witnesses the emergence of further keywords: *structure sensitivity* and *carbon nanohorn*.

#### **5.4.3. Biotechnology and Biomedicine: Therapeutic biomedicine – purple cluster**

In 2010, Germany exerted greater specialization in the research topic *arabidopsis protein*, whereas *lipid nanocapsule* has a higher presence in France, and *biomedicine* prevails in Spain with *polyanhydride*, *zein* or *biosensing systems*.

In 2014, the keywords *magnetospirillum* and *nanoparticle uptake* cover the focus of most research activity in Germany; *lipid nanocapsule* still shows the highest relative advantage in France, and *caco 2* and *plasmodium* predominate in Spain.

In 2018, *magnetospirillum gryphiswaldens* still evokes the highest research activity in Germany, together with terms such as *orodispersible films* and *tautomerizations*; in France, new terms including *hippocampal neuronal culture* or *chromosome segregation* reflect a surge in research activity; while in Spain *plasmodium*, *brain edema*, *biochemical engineering* or *parkinsonism* emerge to represent specialization in NST.

#### **5.4.4. Physical and mechanical characteristics of nanomaterials – blue cluster**

The evolution of this research topic in 2010 is highly specialized in *meristem* and *magnetic* in Germany. In France, specialization is concerned with *yarn* and *nanobiocomposite*. In Spain, the highest degree of research activity is

initially represented by *water vapour permeability* and *nanostructured ceramic*.

In 2014, terms reflect lesser research efforts in Germany, when relative advantages surrounded terms such as *scanning force microscopy* or *miniemulsion*. France's research activity revolves around terms such as *hydrophobic molecule*, *polyelectrolyte multilayer film* or *supramolecular organization*. In Spain, terms such as *nanohydrogel* and *sepiolite* underline intensified research efforts.

In 2018, NST German efforts are focused on *invertebrate* or *stable isotopes*. In France, specialization shifts to *polyoxometalate* or *diagenesis*. *Sepiolite* still indicates high activity in 2018, together with *mytilus* and *smectite* in Spain

#### **5.4.5. Biotechnology and Biomedicine: Biosensing – orange cluster**

In 2014, research related to *Biosensing* displays the highest specialization through keywords such as *enbucrilate* and *fluorescence lifetime imaging microscopy* in Germany; *intravenous injection* shows intensified research activity in France; in Spain, the keyword *hyperthermia applications* reflects the most NST activity.

In 2018, this research topic shows different specialized terms. For example, in Germany *phenyleneethynylene* and *photoswitch* mark the highest research activity; in France, the keywords are terms such as *multivalency*, *chiral* and *polyelectrolyte multilayer*; and in Spain, *biomedical analysis* or *thermo sensitive polymer* are the terms designating the most intensive research activity.

#### **5.4.6. Biotechnology and Biomedicine: Regenerative medicine – light yellow cluster**

In 2014, Germany put emphasis on the term *synthetic bone graft*. In France, keywords *bisphosphonates* and *cortical bone* display the highest research

activity. Spain's research activity is more focused on *saliva substitute* and *remineralization*.

In 2018, Germany's terms reflecting the highest relative advantages are *zoledronic acid* and *periosteum*. In France, new terms emerging are *bone mineral*, *bicuspid*, *physico chemical and mechanical property*. In Spain, *saliva substitute* and *artificial saliva* still show activity, but a bit less than in 2014. The emergent terms denoting new and intensive research activity would be *hydroxyapatite nanorods* and *physico chemical and mechanical property*.

## **6. Discussion**

This study provides an overview of the cognitive structure and the relative specialization or comparative advantage of countries at the level of publications and research topics over time in NST research. We analyzed relative strengths and weaknesses in national performance and international competitiveness. The focus is an international comparison for three European countries (Germany, France and Spain) against a world baseline. This overview proves how mapping knowledge and depicting scientific intellectual structures in NST (or any other knowledge domain) are of importance to understand how research develops and how research units relate to each other in a given domain. When provided with an intuitive "picture," it is easy for informetricians, research assessors, and even the public at large to discover a domain's inner structure and extract key clusters [58].

Our results reveal changes in the cognitive structure of NST at the global level, with new research topics popping up here and there. NST research tends to explore new technologies and applications holding potential to address societal challenges, improve the quality of life, and optimize industries that might benefit society, a finding in consonance with previous studies [59,60]. Porter et al. [18] argue that the development of theoretical stages in this domain helps consolidate new research topics focused on

concrete applications of NST theories, which witnessed remarkable developments in engineering, medical and biological areas of NST. The novelty of this paper is that we show differences in national cognitive structures. For example, we observe that Germany's scientific research is more concentrated on *Biotechnology and Biomedicine* research topics and *Microelectronics engineering and top-down processes* than France or Spain, at the world baseline. Within France, *Biotechnology and Biomedicine: Therapeutic biomedicine* is well represented, although the other research topics do not suggest noteworthy strength with respect to the world. *Physical and mechanical characteristics of materials* (blue) output is lower in Spain than in Germany or France, but the frequency of occurrence of its terms increases more at the world baseline. Such differences may reflect diverse institutional settings and hence management cultures [61,62]. Further study is needed to explore how such factors may influence a country's output and competitive edge. The analysis presented here, highlighting the strengths of particular countries, is helpful to orient research in certain fields to gain or maintain a firm research position, create alliances or collaborative ties with other countries, or compensate for weaknesses detected.

Overall, NST publications have undergone vast development over the last decade, as evidenced by the cumulative number of publications at a worldwide level. Notwithstanding, the growth is unevenly distributed among countries. For example, while the number of publications in Spain is still lower than in Germany or France, its growth in the past decade is greater (SI, Tables S1 and S2). This growth does not correspond with the rate of specialization, meaning that while Germany and France show some degree of specialization with respect to the world in the early years of study, their specialization decreases when the output in NST grows at a faster pace in other countries, for instance Iran or South Korea. Specialization profiles in core NST research may be high despite a relatively low world share (see SI, Table S3). The dynamics of scientific output in every single country and

interactions among countries worldwide are both determinant factors behind advances in NST or other fields of specialization.

Some countries perform more or less evenly in terms of output and specialization, whereas others have evident and characteristic core strengths, even in research topics where the relative investment is low [63,64]. This can be quantified in various ways. For example, the specialization index applied by Chinchilla-Rodríguez et al. [45] showed Asian countries to have a higher concentration of NST research output than the rest of the studied countries, a possible indication that NST research has become established as a scientific priority in this geographical area. In contrast, though the United States is the greatest producer overall, it stands out only in specialization in 2003 with an excellence rate above the world average. France is the 6th greatest producer of NST, with a specialization index above the worldwide level, but its excellence rate is below the global average. Institutional settings and research management may play a key role in these outcomes; further analysis is needed to explore this possibility.

In short, each country (or geographical area) shows a different pattern of specialization based on NST publications, which is a potential signal of relative advantage with respect to collaborators or competitors at the worldwide level. According to Hidalgo et al. [65], in terms of “product space”, these results may have important implications for economic policy, because they point to topics where a country might promote efforts toward transformation and gaining an upper hand within a specific scientific field. Such efforts could be focused, for example, on the economic investment to be made for products (topics) of vast potential, bearing in mind the level of a country and its weight in the global realm. When economic resources destined to the sciences are scanty, knowing just what and how countries produce can be determinant for allotment. As stated by Adams [62], even if the frontiers of research are endless, each country has only a limited quantum of good

research to offer. Investment beyond that point is nugatory; greater quantity inevitably means poorer quality.

Despite the challenges involved, the ultimate aim is to ensure greater efficacy in the development of research and sound competition in the global realm, including collaborative efforts among different countries, aspiring to “Smart specialization”. This term refers to a political framework of vertical orientation that reflects the priorities established at a regional level. It combines upward and downward dynamics to set priorities for public investment in knowledge. This strategy helps guarantee that governmental efforts and resources are not spread out evenly; the key question is how to select the most relevant areas deserving investment [66]. Such a diagnosis foments positive transformation, by updating neglected areas, advancing along new lines of interest, or fortifying areas already competitive at the international level. Smart specialization entails identification of national strengths and weaknesses within research fields to establish priorities accordingly. It may be a useful strategy for building scientific capacity in developing and peripheral countries [67]. Alternatively, nations may develop a consensus about investment, and develop programs to concentrate talent behind core.

There are some limitations regarding this study that should be mentioned. First, the analysis and comparison of just a few European countries is an obvious geographical limitation. Still, this approach could be extended to analyze any country or institution in further efforts, to study a broad set of countries across continent and/or scientific capacities [68]. Second, the results point to variations among the years under study, meaning we cannot affirm whether the results would have been different if other years had been chosen. That is, our findings apply only to the specific years under study. Therefore, the results should be considered with caution under the focus of the particular countries and two dimensions of analysis applied in this exploratory research effort. Third, criticism of the Activity Index and its mathematical equivalents might be a limitation. AI implies entails some

theoretical problems due to its mathematical structure [69], and its values for one field could be affected by the output activity of other countries and fields, so that an across-field comparison would be misleading [70]. Interpreting the results obtained using these indicators in the realm of science calls for some caution [41]. And lastly, we use high-frequency keywords to illustrate the combination of co-word analysis and activity index. Other non-high frequency keywords might be selected in further studies to unveil and compare research advantages possibly leading to innovative NST research if these keywords appear in all units of analysis (countries, institutions, etc.) [39,42].

In addition, for a more detailed analysis of NST research, approaches involving broader coverage (see for example, Hook et al. [71] and Huang et al. [72]) could be undertaken. Alternative data sources would enrich analysis—for example, considering the ration of qualified personnel with respect to the total population, or the sectors most involved in knowledge production (namely, industry, government, or higher education sectors).

In sum, this approach or any other approach can always be subjected to debate. Its suitability for a broad array of fields suggests a diversity of outcomes that might serve as feedback to modify and/or improve its application, in search of a process that will lead us closer to consensus among the scientific community. The methodology suggested in this study is therefore not limited to the EU countries or domain chosen, but can be extrapolated to 1) other countries; and 2) further domains. It was designed as is presented as an assay under proof. Testing this method is by no means exhaustive; here the focus of analysis included Spain, but other countries could just as well have been chosen. Likewise, not only researchers but also policy managers and information professionals might find this method useful to explore a variety of countries and domains. Further work is needed to provide indicators and interpretations of NST that would contribute to a more profound understanding of how research is produced, shared and developed.



## 7. Conclusion

Despite the aforementioned limitations, this research paper and the results it projects can be seen as a platform of evidence to support decision-makers when developing new policies that favor smart specialization and good practices in scholarly communication. The analysis of research topics is relevant because it substantiates the link between scientific yield in terms of the effort and level of activity undertaken by countries against a world baseline, and brings to light relationships within the competitive structure of a domain. The combination of several techniques may be applied for technological surveillance in economic research policy and technological development. Future studies could attempt to untangle these associations at higher (regions) or lower levels (institutions) of aggregation. A global benchmarking analysis would help us gain a holistic view of knowledge production and the scientific capacities of countries, sectors or institutions.

In conjunction with the research aims stated, our contribution is twofold. Firstly, we trace the cognitive structure of NST over time by updating the NST dataset as described by Muñoz-Écija et al. [12]. This comprehensive search strategy along with science mapping provides an opportunity for a full grasp of NST development, while also proving useful to quickly detect relevant research. Secondly, our modification of the AI to measure keywords helps determine the salient research topics of countries. This modification can enhance the characterization of a national or regional profile, so as to detect efficiency in terms of specialization/innovation, in a field within the overall context of research output. Shedding new light on the background and characteristics of a domain could aid researchers in their own development and potentially support collaborations, calls for grants, or mobility programs. Therefore, having this information essentially “at a glance” may accelerate investment along strategic research topics, which is beneficial for all the parties involved.

## **Authorship contribution statement**

Author 1: Conceptualization, Methodology, Data Curation, Formal analysis, Writing- Original Draft, Writing- Reviewing and Editing.

Author 2: Methodology, Software, Writing- Reviewing and Editing, Visualization, Supervision

Author 3: Conceptualization, Methodology, Writing- Original Draft, Writing- Reviewing and Editing, Supervision

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## **Declaration of conflicting interests**

None of the authors has a conflict of interest to declare.

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## Supplementary Information

### Supplementary text S1. Search strategy for Scopus database

<https://data.mendeley.com/datasets/p9rtkcm93c/1>

### Supplementary text S2. Thesaurio

<https://data.mendeley.com/datasets/p9rtkcm93c/1>

**Table S1. Total number of NST publications and share world output for the most prolific countries 2010, 2014 and 2018**

	Nano Output				Total Output			Npub (%)		
	Total	2010	2014	2018	2010	2014	2018	2010	2014	2018
United States	428,968	22,534	25,621	25,890	609,632	676,011	705,258	3.70	3.79	3.67
China	427,147	19,893	37,034	54,496	344,556	491,159	608,425	5.77	7.54	8.96
Japan	168,009	7,534	8,025	7,559	130,234	133,048	135,893	5.78	6.03	5.56
Germany	144,550	7,322	8,584	8,558	154,710	175,515	185,992	4.73	4.89	4.60
India	104,478	4,405	9,746	14,779	81,516	133,048	180,049	5.40	7.33	8.21
South Korea	98,844	5,565	7,653	8,025	61,490	79,625	86,852	9.05	9.61	9.24
United Kingdom	94,612	4,672	5,933	6,802	176,759	200,574	219,189	2.64	2.96	3.10
France	94,103	4,818	5,631	5,517	108,703	121,868	124,646	4.43	4.62	4.43
Russian Federation	72,333	3,103	4,555	7,242	40,703	58,904	104,389	7.62	7.73	6.94
Italy	61,562	3,057	4,321	4,685	87,609	109,640	123,521	3.49	3.94	3.79
Iran	51,237	1,987	5,141	8,536	30,105	45,719	59,818	6.60	11.24	14.27
Spain	50,251	2,780	3,808	4,124	73,970	91,144	98,227	3.76	4.18	4.20
World		96,605	136,731	162,914	2,466,831	2,929,527	3,207,087	3.92	4.67	5.08

NPub (%): World NST publications share

**Table S2. Growth rate, mean average growth rate (MAGR) and ratio for the most prolific countries 2010, 2014 and 2018**

	Nano Growth Rate		MAGR	Total Growth Rate		MAGR	RATIO
	2010-2014	2014-2018	2010-2018	2010-2014	2014-2018	2010-2018	
United States	13.70	1.05		10.89	4.33	7.61	0.00
China	86.17	47.15	66.66	42.55	23.88	33.21	2.01
Japan	6.52	-5.81	0.36	2.16	2.14	2.15	0.17



Germany	17.24	-0.30	8.47	13.45	5.97	9.71	0.87
India	121.25	51.64	86.45	63.22	35.33	49.27	1.75
South Korea	37.52	4.86	21.19	29.49	9.08	19.28	1.10
United Kingdom	26.99	14.65	20.82	13.47	9.28	11.38	1.83
France	16.87	-2.02	7.42	12.11	2.28	7.20	1.03
Russian Federation	46.79	58.99	52.89	44.72	77.22	60.97	0.87
Italy	41.35	8.42	24.89	25.15	12.66	18.90	1.32
Iran	158.73	66.04	112.38	51.87	30.84	41.35	2.72
Spain	36.98	8.30	22.64	23.22	7.77	15.49	1.46
World	41.54	19.15	30.34	18.76	9.47	14.12	2.15

**Table S3. Activity Index and Relative Specialization Index NST for the most prolific countries 2010, 2014 and 2018**

	AI			RSI		
	2010	2014	2018	2010	2014	2018
United States	0.94	0.81	0.72	-0.03	-0.10	-0.16
China	1.47	1.62	1.76	0.19	0.24	0.28
Japan	1.48	1.29	1.10	0.19	0.13	0.05
Germany	1.21	1.05	0.91	0.09	0.02	-0.05
India	1.38	1.57	1.62	0.16	0.22	0.24
South Korea	2.31	2.06	1.82	0.40	0.35	0.29
United Kingdom	0.67	0.63	0.61	-0.19	-0.22	-0.24
France	1.13	0.99	0.87	0.06	-0.01	-0.07
Russian Federation	1.95	1.66	1.37	0.32	0.25	0.15
Italy	0.89	0.84	0.75	-0.06	-0.08	-0.15
Iran	1.69	2.41	2.81	0.26	0.41	0.47
Spain	0.96	0.90	0.83	-0.02	-0.06	-0.09
World	1.00	1.00	1.00	0.00	0.00	0.00

**Data S1. KAI and RSIk in 2010 (Germany-France-Spain)**

<https://data.mendeley.com/datasets/p9rtkcm93c/1>

**Data S2. KAI and RSIk in 2014 (Germany-France-Spain)**

<https://data.mendeley.com/datasets/p9rtkcm93c/1>

**Data S3. KAI and RSIk in 2018 (Germany-France-Spain)**

<https://data.mendeley.com/datasets/p9rtkcm93c/1>

## Lista de siglas y acrónimos

2D	Dos Dimensiones
3D	Tres Dimensiones
AI	Activity Index
CAB	Citation-Assisted Background
CENIT	Centro para el Desarrollo Tecnológico e Industrial
CWTS	Centre for Science and Technology Studies
DOMINO	Desarrollo y Obtención de Materiales Innovadores con Nanotecnología Orientada
EPO	European Patent Office
FP	Framework Programmes for Research and Technological Development
GR	Growth Rate
H2020	Horizonte 2020
I+D+i	Investigación, Desarrollo e Innovación
ISI	Institute for Scientific Information
JCR	Journal Citation Reports
KAI	Activity Index based on Keywords
MAGR	Mean Average Growth Rate
MDS	Multidimensional Scaling
NBIC	Nanotechnology, Biotechnology, Information Technology and Cognitive Science
NNI	National Nanotechnology Initiative
NST	Nanoscience and Nanotechnology
N&N WC	Nanoscience and Nanotechnology WoS Category
OCDE	Organisation for Economic Co-operation and Development
OLS	Ordinary Least Squares
RSI	Relative Specialization Index
RSIk	Relative Specialization Index based on Keywords
SCI	Science Citation Index
SCI-EXPANDED	Science Citation Index Expanded
SIR	Scimago Institutions Rankings
SJR	SCImago Journal & Country Rank
SSCI	Social Sciences Citation Index
UE	Unión Europea
USPTO	United States Patent and Trademark Office
WIPO	World Intellectual Property Organization
WoS	Web of Science

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## TESIS DOCTORAL

### DELIMITACIÓN DE CATEGORÍAS CIENTÍFICAS EN BASES DE DATOS MULTIDISCIPLINARES: NANOCIENCIA Y NANOTECNOLOGÍA COMO ESTUDIO DE CASO

Teresa Muñoz Écija

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9	2	7	FlexRoom	Flex Room
9	4	3	marbellís	marbellíes
11	1	5	categoría	categorías
19	1	13	Unión Europa	Unión Europea
23	3	6	descubrimiento microscopio	descubrimiento del microscopio
20	2	5	Commision	Commission
26	2	6	Commision	Commission
26	4	1	en cabo	a cabo
27	1	4	o a	y a
31	1	2	primera	primeras
33	2	2	de dominios científico:	de dominios científicos:
41	2	10	de la citas	de las citas
42	3	1	Los publicaciones	Las publicaciones
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48	5	2	científica,	científica
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54	3	6	desarrollo y	desarrollo e
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57	2	1	Análisis de los	Analizar los
63	2	6	de total documentos	total de documentos
65	2	1	Wos	WoS
65	3	1	identificaron	identificaron
65	3	7	dimensión citante	dimensión citada
75	3	1	Fleiss's kappa	Fleiss' kappa
83	2	9	número publicaciones	número de publicaciones
84	2	3	detectarse hasta	detectar hasta
97	4	6	loose	lose
107		28	European Commision	European Commission
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209	2	2	Fleiss's kappa	Fleiss' kappa
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