

2D-Materials based memristors for neuromorphic computing



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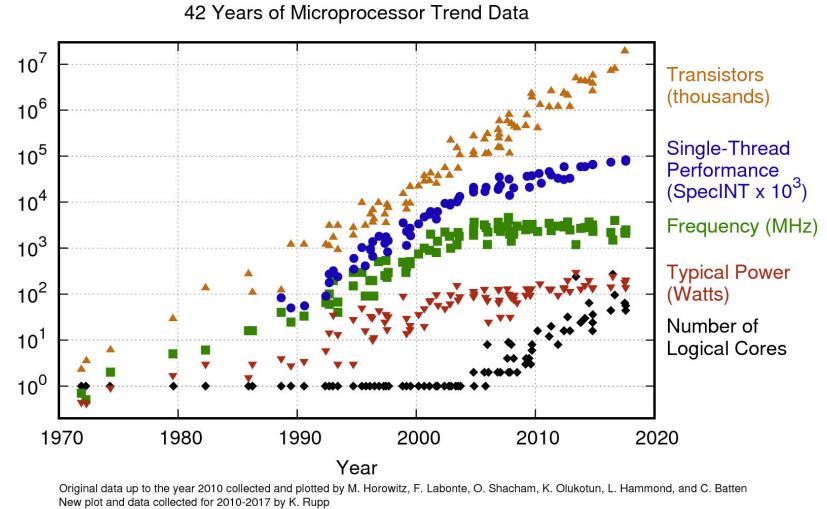
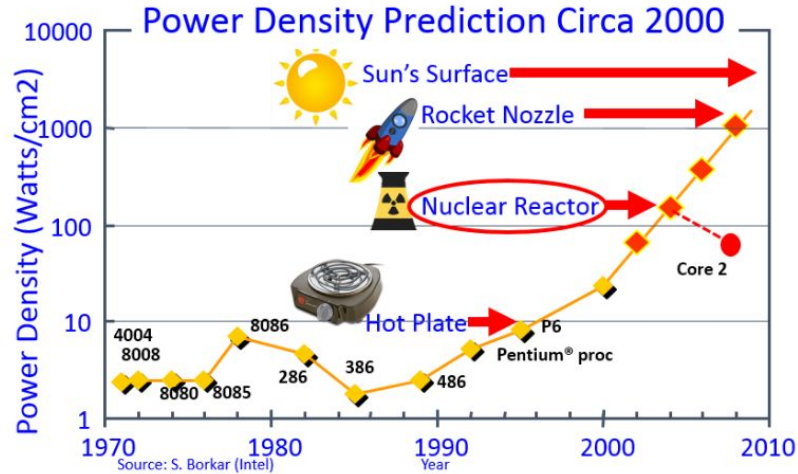
Mari-Carmen Pardo

Roberto Motos

Mari-Carmen Fernandez

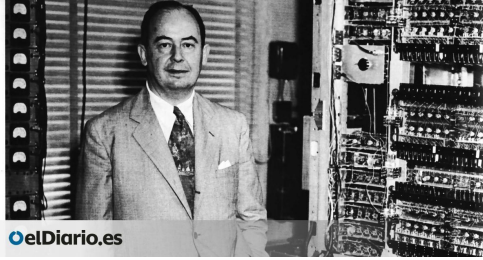
Mikel Garcia

There is no free lunch !!

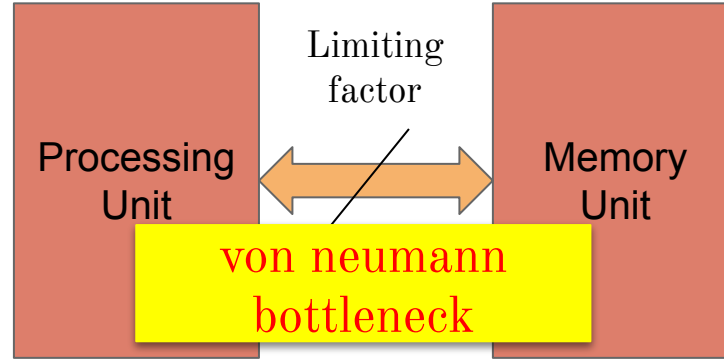
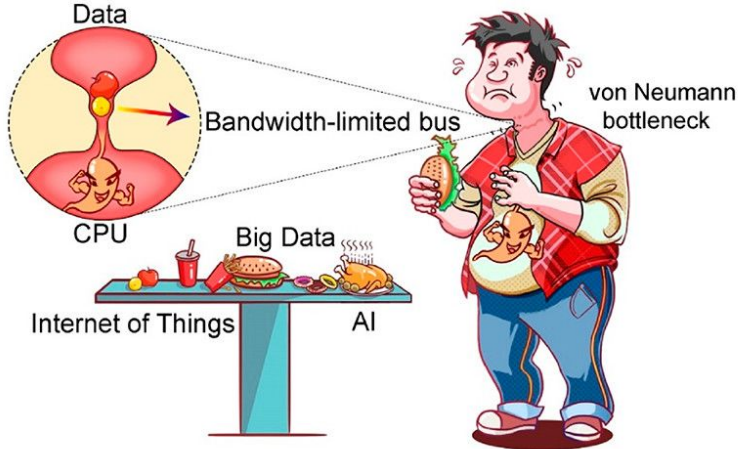


Power density is the limiting factor

Where does the energy goes ?



John von Neumann



Processing and memory unit are physically separated



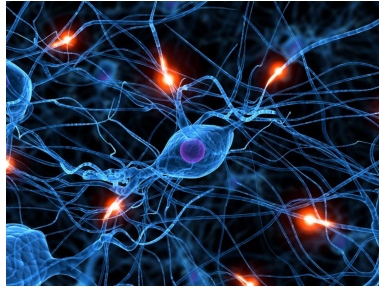
Inspiration is right here !!

The most power efficient machine

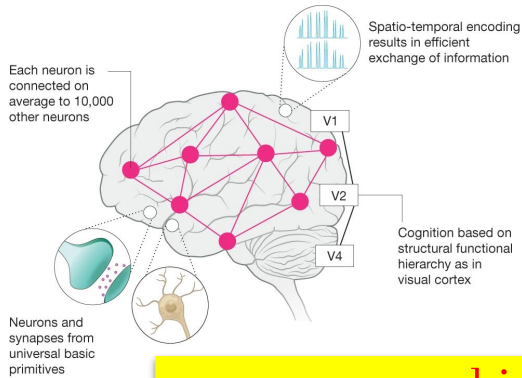


~ 20 W

G. J. Siegel, et. al.
Lippincott-Raven, 1999



non von Neumann architecture

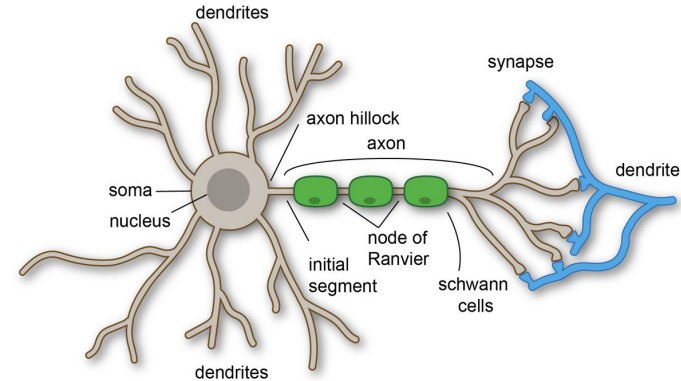


Roy, K., et. al., *Nature*, 2019

10^{11} neurons

10^{15} synapses

neuromorphic computing



Need electronic equivalent of biological synaps

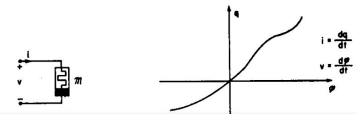
Memristor - an entelechy

Memristor—The Missing Circuit Element

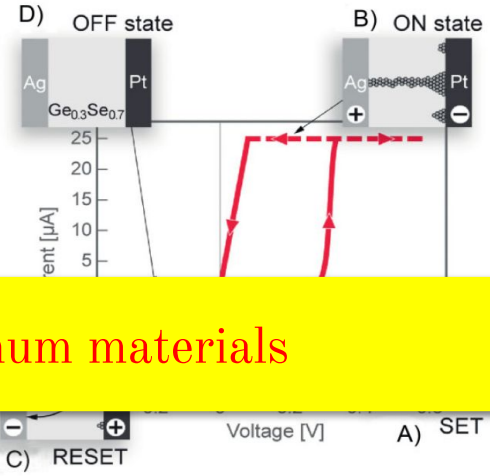
LEON O. CHUA, SENIOR MEMBER, IEEE



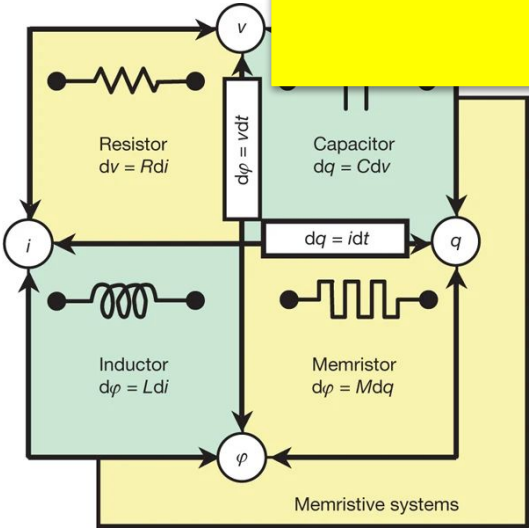
ent—called the memristor—
charge $q(t) \equiv \int_{-\infty}^t i(\tau) d\tau$
introduced as the fourth basic
iteration of this relationship
all's equations is presented.
rs are derived. It is shown
behavior different from that
. These properties lead to a
: be re



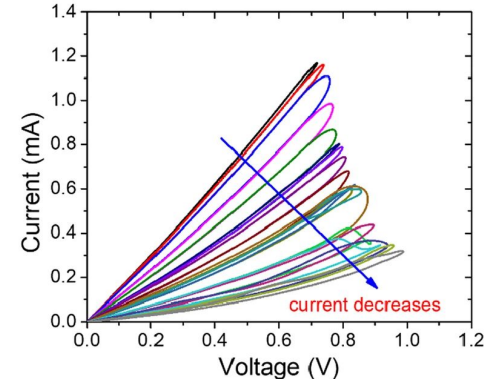
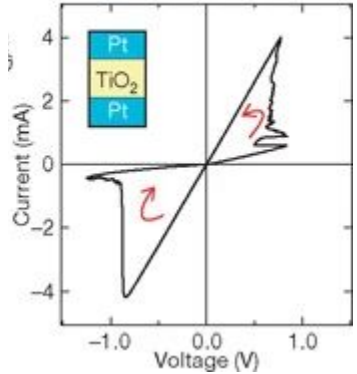
Ongoing hunt for optimum materials



Waser, Rainer, et al.,
Advanced materials
2009.

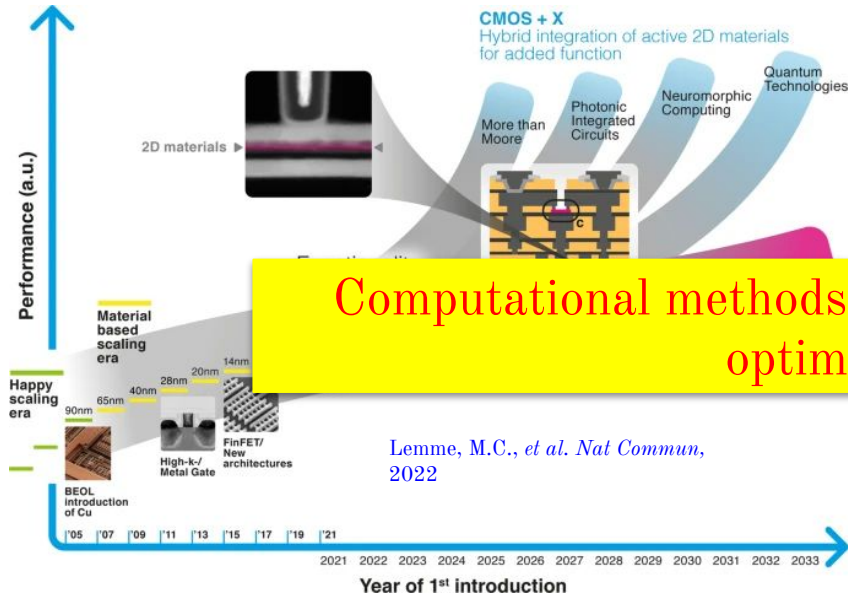


Strukov, D., et al. *Nature* 2008



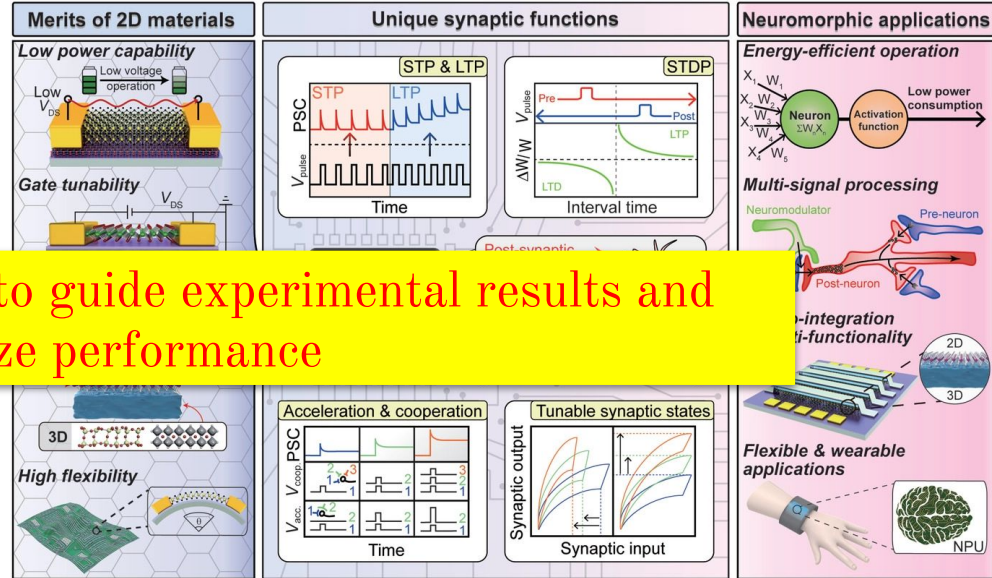
Ismail, M. et al.
Nanoscale Res Lett,
2022

2D Materials - paradigm shifting discovery



Computational methods to guide experimental results and optimize performance

Lemme, M.C., et al. *Nat Commun*, 2022



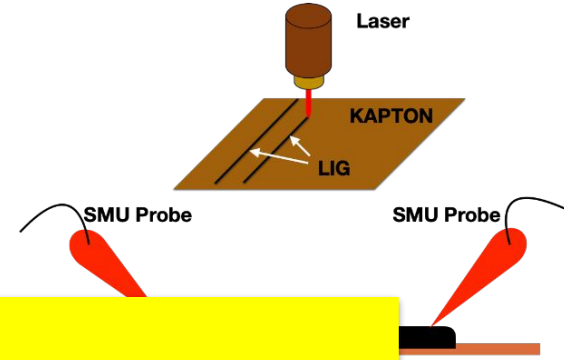
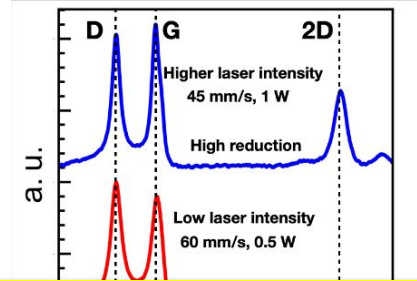
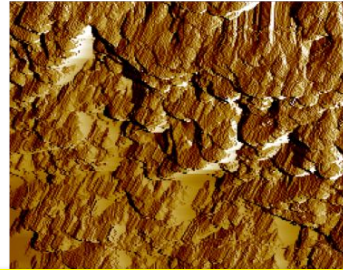
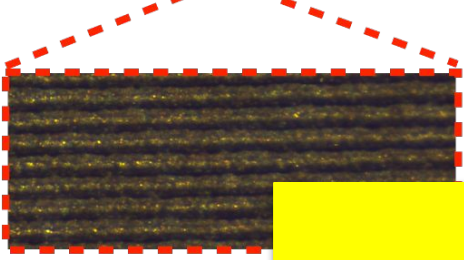
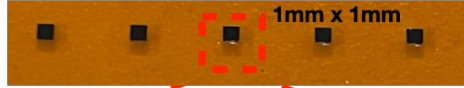
Huh, Woong, et al., *Advanced Materials*, 2020.

Fundamental challenges remains -

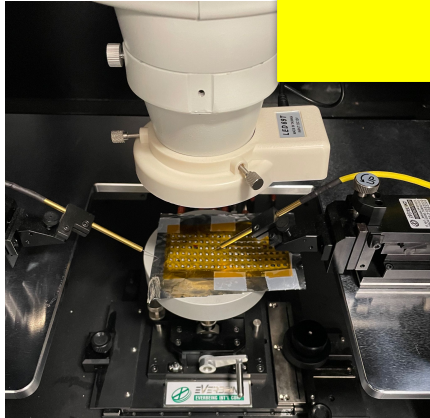
- Large scale fabrication
- Endurance
- Retention time
- Which material and mechanism

Memristor Fabrication at University of Granada

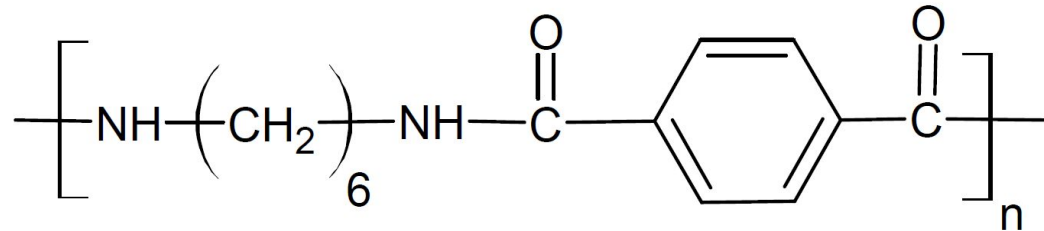
Laser Induced Graphene



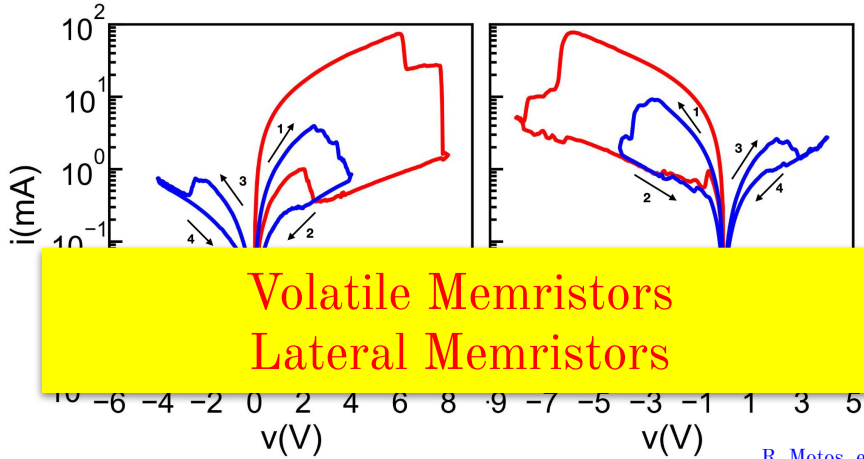
Low Cost Process
Flexible Substrate



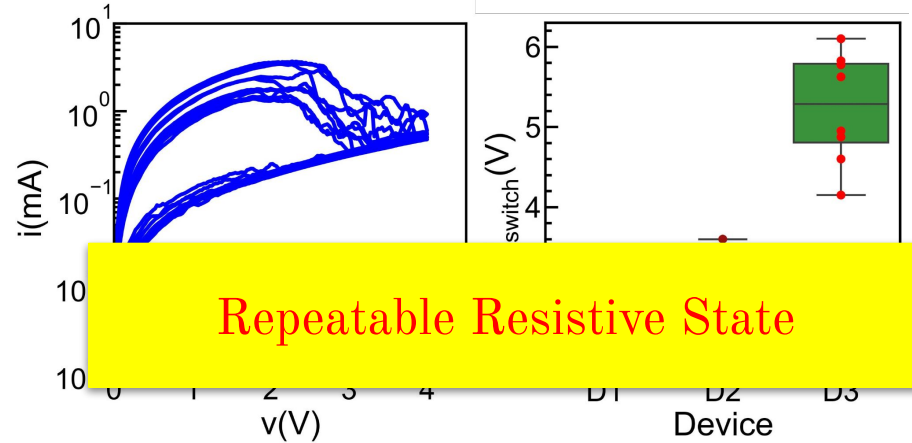
Polyamide



Memristor Fabrication at University of Granada

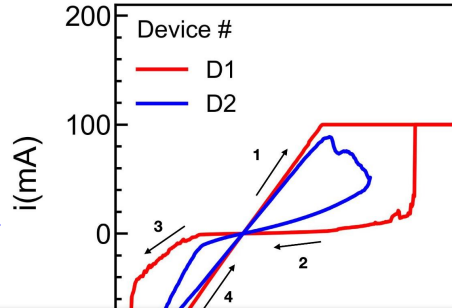


Volatile Memristors
Lateral Memristors



Repeatable Resistive State

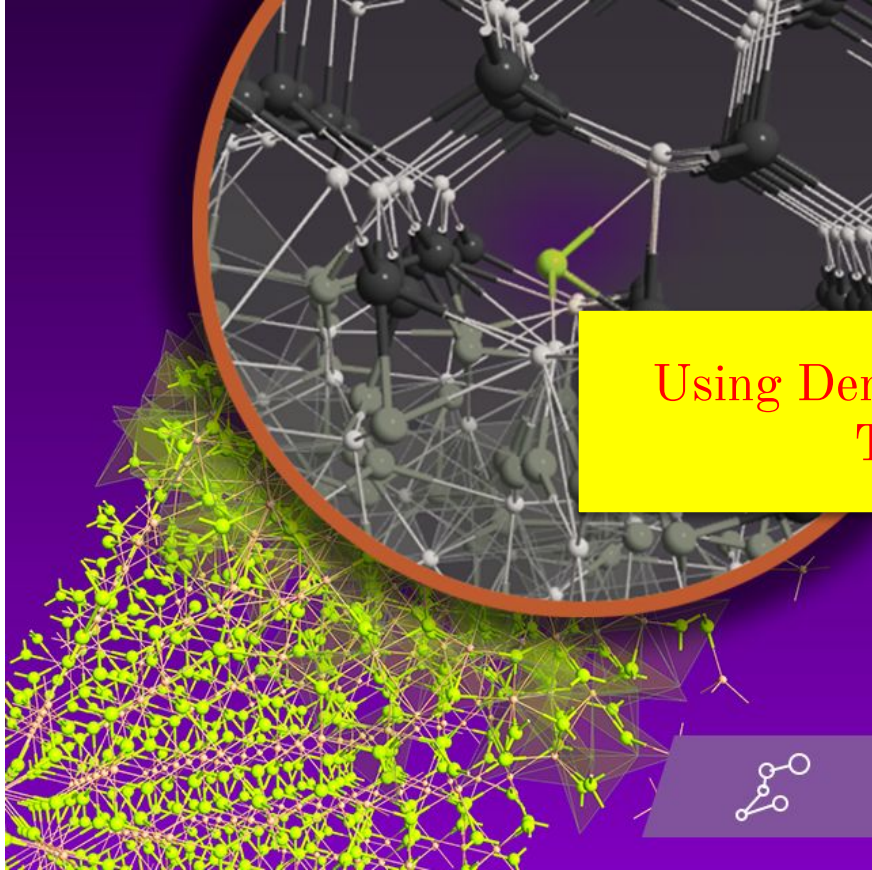
M. Fernandez. et. al., CDE, 2023 (submitted)



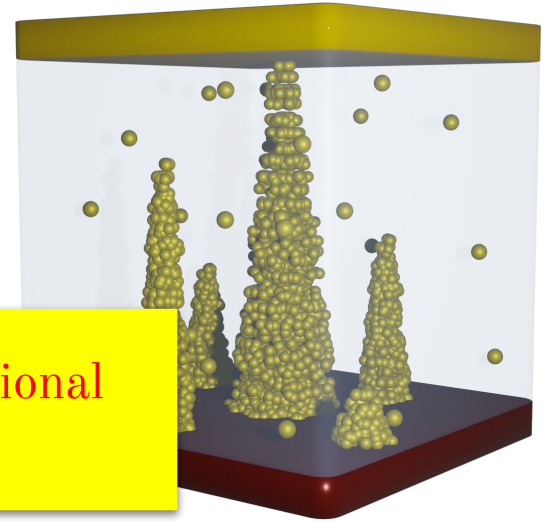
Non-Volatile Memristors
Vertical Memristors

R. Motos et. al., DRC, 2023 (submitted)

Ab initio simulations

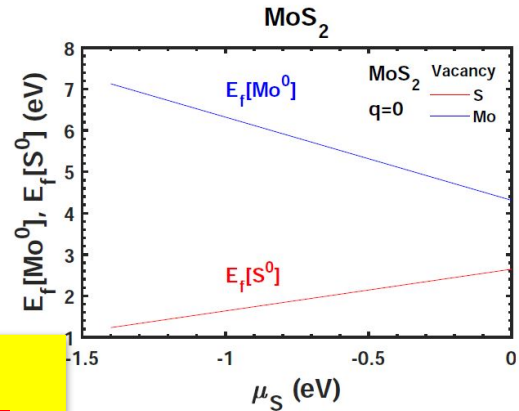
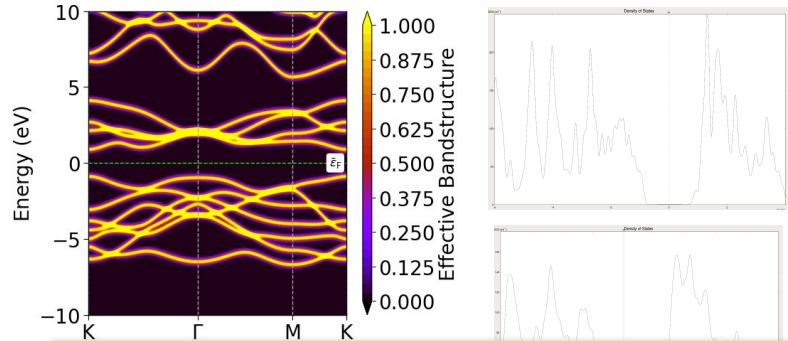
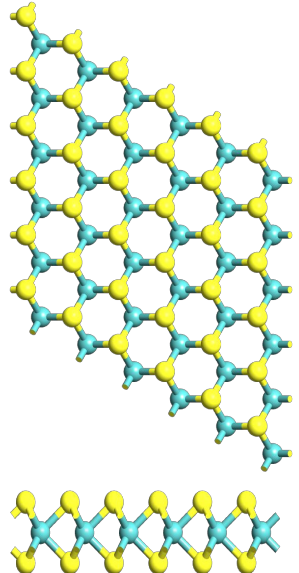


Using Density Functional
Theory



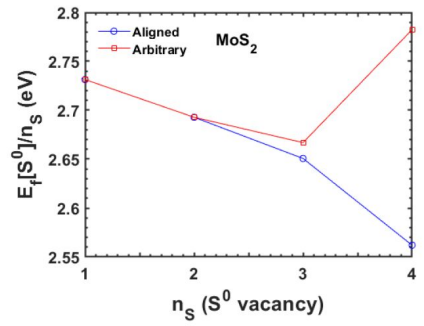
$$\left(-\frac{\hbar^2}{2m} \nabla^2 + v_{\text{eff}}(\mathbf{r}) \right) \varphi_i(\mathbf{r}) = \varepsilon_i \varphi_i(\mathbf{r}).$$

Ab initio simulations



Thermodynamically stable defect - types and position

$$E_{tot}[bulk] - \sum_i n_i \mu_i + q(E_{VBM} + \mu_e) + E_{corr}$$

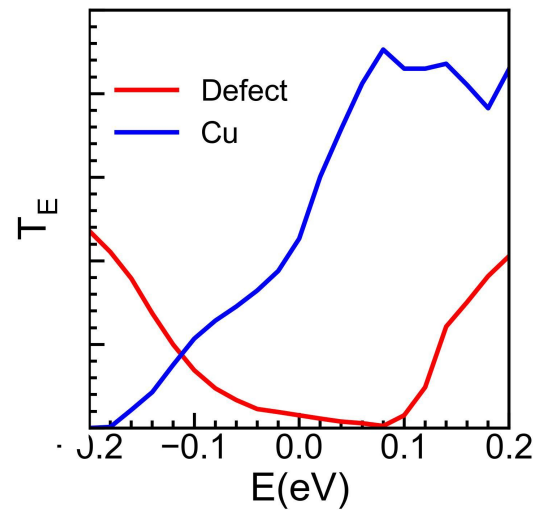
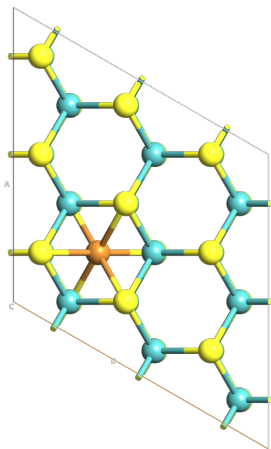
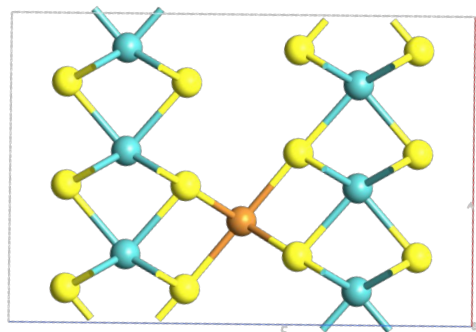
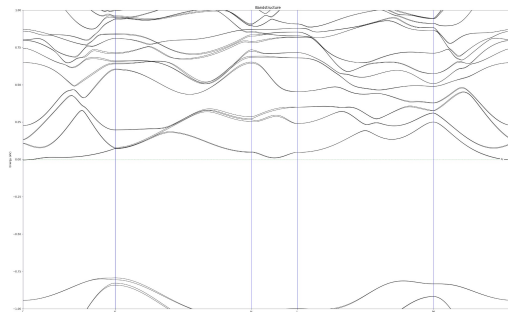
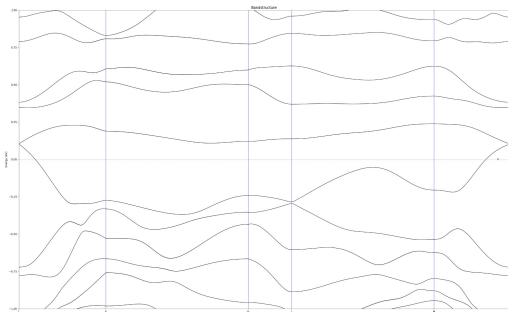
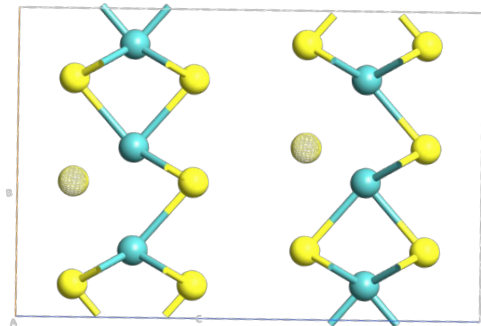


n_S	Aligned (eV)	Arbitrary (eV)
1	2.73	2.73
2	2.69	2.69
3	2.65	2.66
4	2.56	2.78

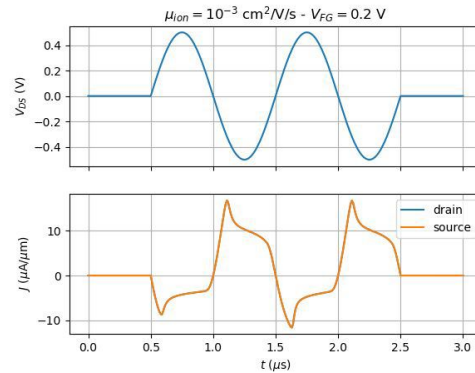
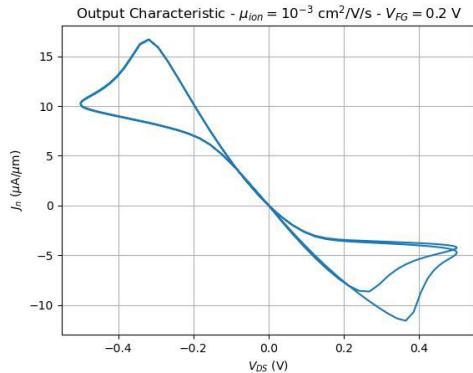
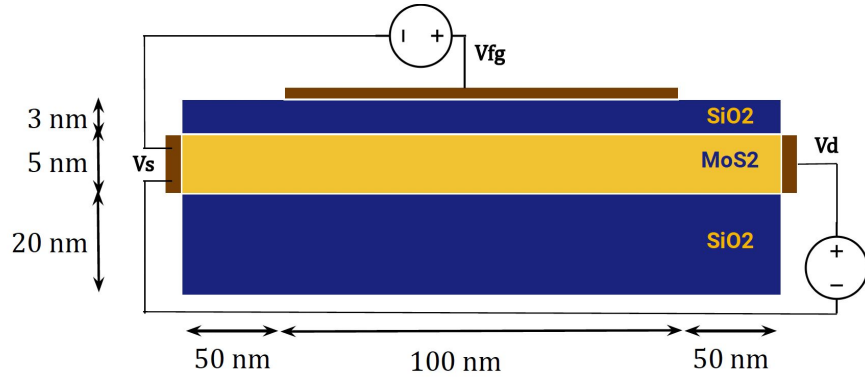
Crystal	Y Vacancy	E_f (eV)
PtS ₂	S	1.98
PtTe ₂	Te	2.00
PtSe ₂	Se	2.09
WTe ₂	Te	2.21
MoTe ₂	Te	2.39
WSe ₂	Se	2.46
MoSe ₂	Se	2.47
MoS ₂	S	2.64
WS ₂	S	2.70

Crystal	X Vacancy	E_f (eV)
WTe ₂	W	2.75
PtTe ₂	Pt	3.22
MoTe ₂	Mo	3.40
PtSe ₂	Pt	4.39
PtS ₂	Pt	5.23
WSe ₂	W	5.33
MoSe ₂	Mo	5.85
WS ₂	W	6.65
MoS ₂	S	7.12

Transport study using NEGF + DFT



Numerical Simulation



Self-consistent Simulation

$$\vec{\nabla} \cdot (\epsilon \vec{\nabla} V) = -\rho$$

$$n = \int_{-\infty}^{\infty} g(E + V) f(E + V, E_F) dE$$

$$\vec{\nabla} \cdot \vec{J}_n = \vec{\nabla} \cdot \left(\epsilon \frac{\partial}{\partial t} \vec{\nabla} V \right) + \sum_i \frac{\partial c_i}{\partial t}$$

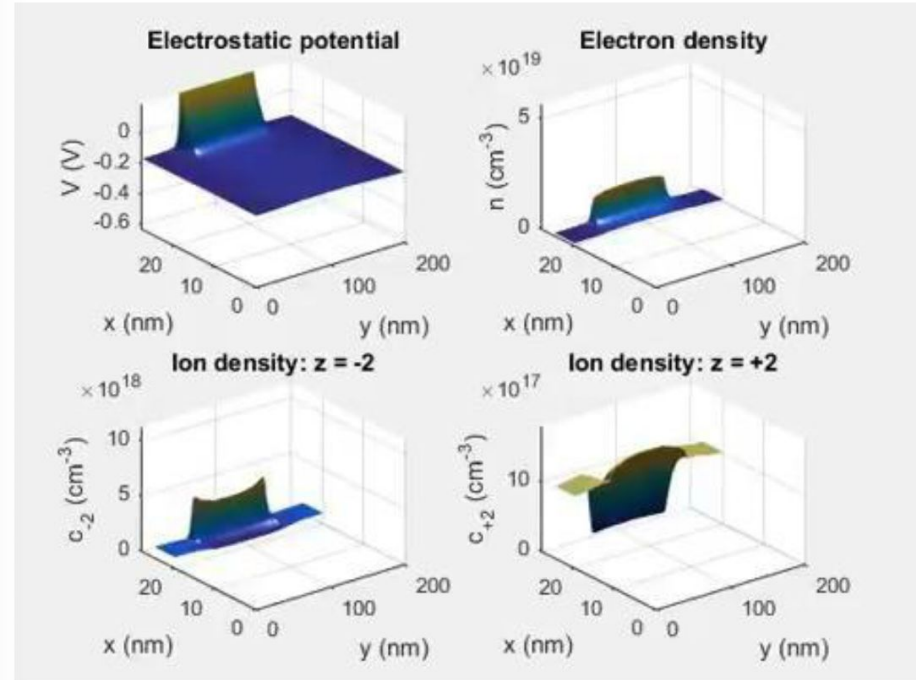
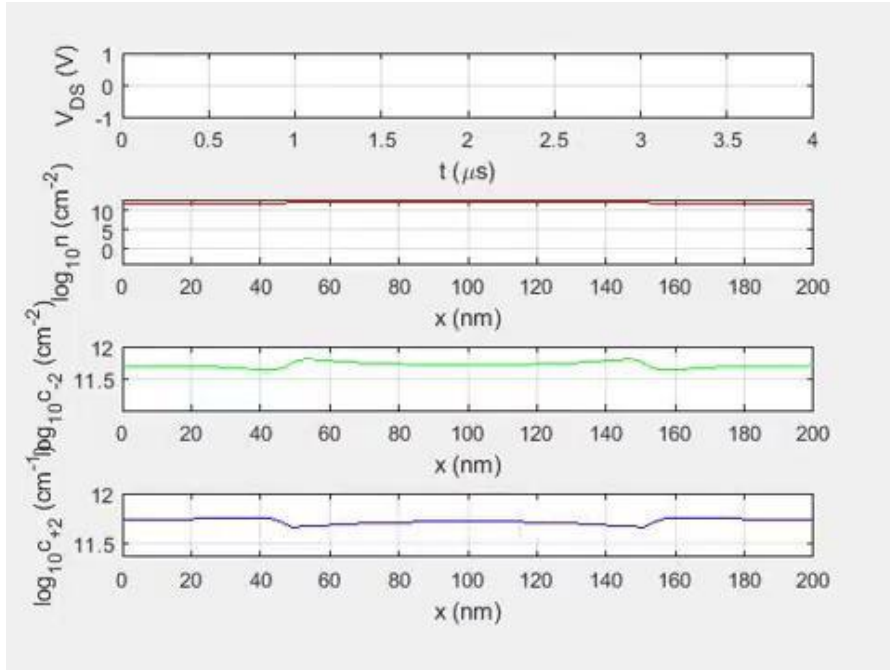
$$\vec{J}_n = q\mu_n n \vec{\nabla} E_{F_n}$$

$$\vec{\nabla} \cdot \vec{J}_{c_i} = -\frac{\partial c_i}{\partial t}$$

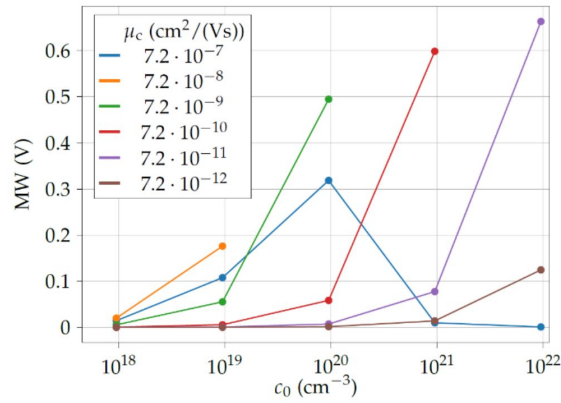
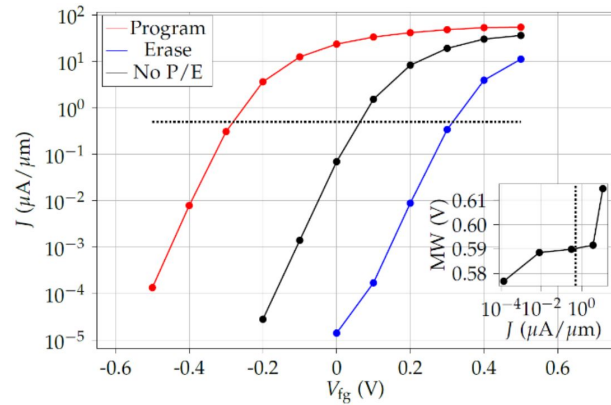
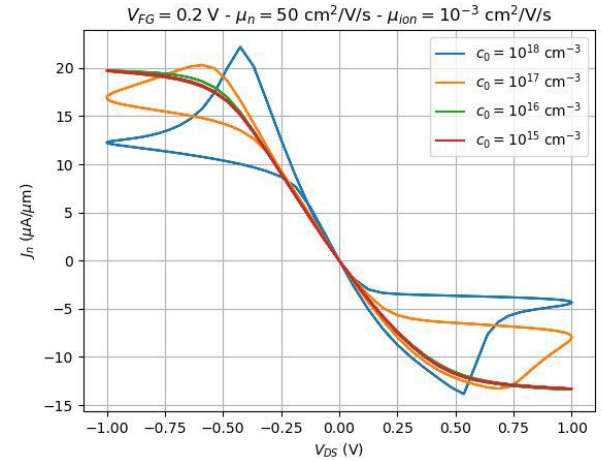
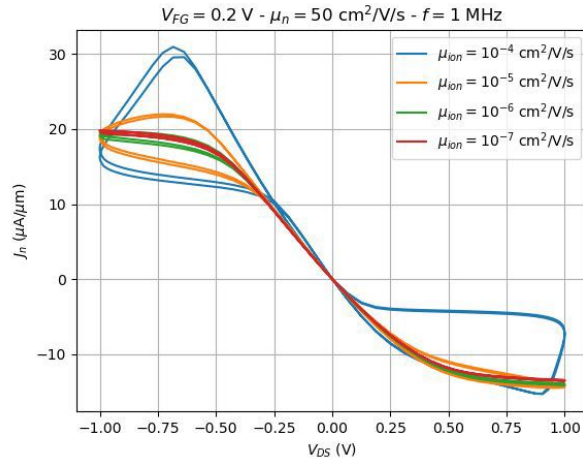
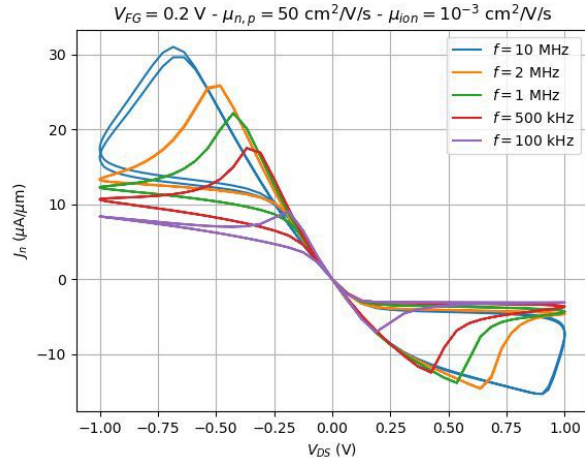
Nerst-Planck:

$$\vec{J}_{c_i} = z_i q D_i \left(-\vec{\nabla} c_i - s_i c_i \vec{\nabla} \frac{qV}{k_B T} \right)$$

Numerical Simulation

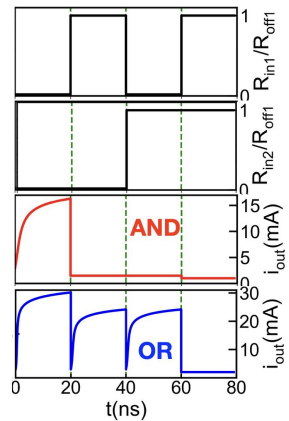
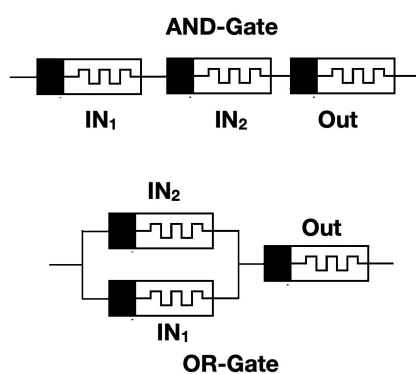
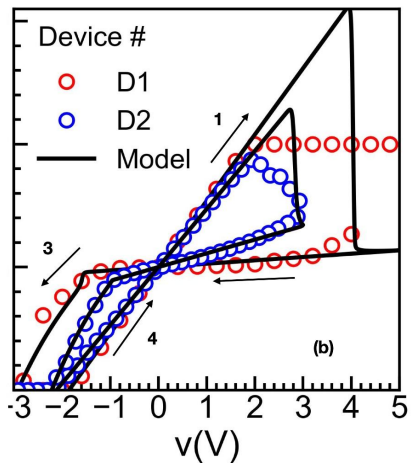


Numerical Simulation



J. Cuesta-Lopez et al., CDE, 2023 (submitted)

Compact Model / SPICE Model

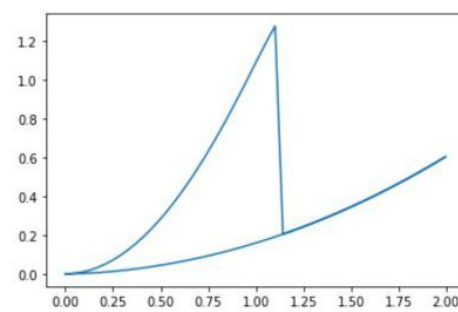
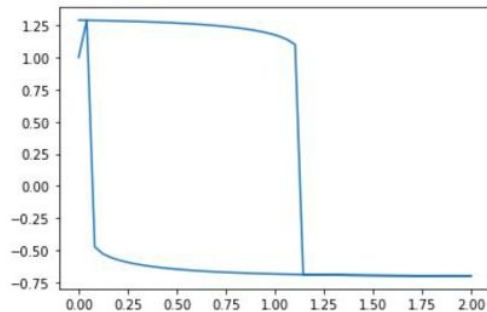
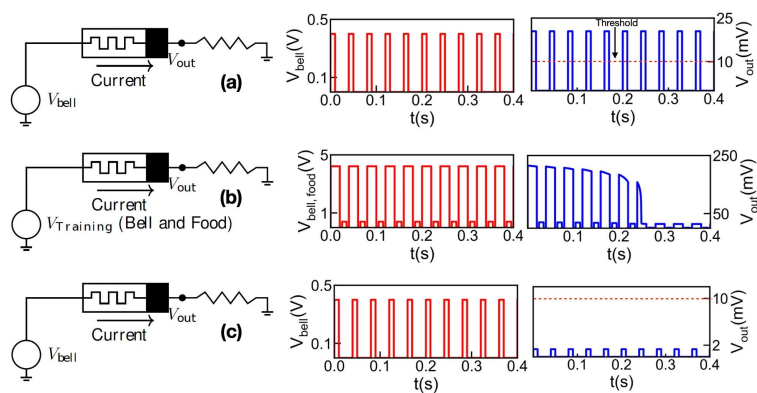


Development of In-house Compact Model

Continuous and cross-compatible

$$I(t) = R * (s(t) + 1) * V^2$$

$$\frac{ds(t)}{dt} = \tanh(-V(t) + 2s(t)) - s(t) + 0.3$$





Thank you



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