Simulation of 2D-material based BioFETs targeting single-molecule detection applications

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Motivation

2D-materials based BioFETs show up as a promising alternative to nanowire based BioFETs, thanks to their higher sensitivity, compatibility with planar technology and easier surface functionalization [1]. Additionally, this technology facilitates the possibility to fully integrate signal processing stages with the sensor.

Methods

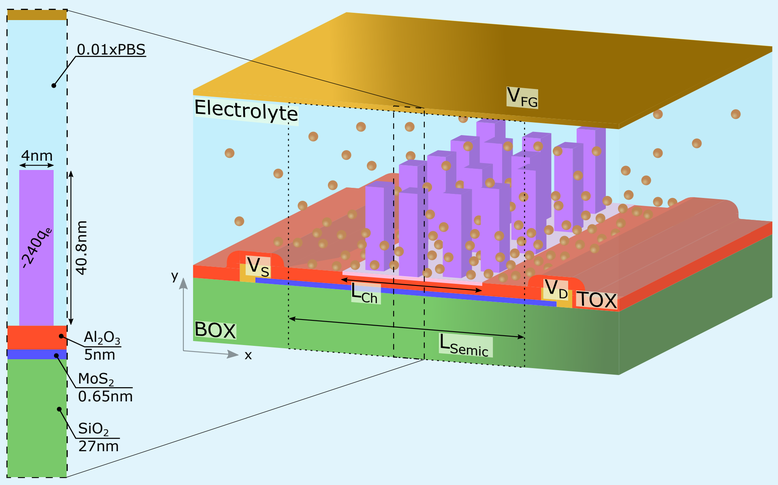
- 2D self-consistent simulation of BioFET [2]:
  - Potential profile in the whole structure:

$$\nabla\left(\epsilon\nabla V\right) = -\rho_{\mathrm{Semic}} - \rho_{\mathrm{Elec}}$$

  - Semiconductor charge: 1D Drift-Diffusion transport with field dependent mobility.
  - Electrolyte (0.01xPBS): simple ions (c_{i}) and phosphate reactions

$$c_i = \frac{c_{i,0}\mathrm{e}^{-qz_i(V-V_{\mathrm{Ref}})/(k_{\mathrm{B}}T)}}{1 - 2\frac{c_{i,0}}{c_{\max}}\left(1 - \cosh\left(q|z_i|\frac{V-V_{\mathrm{Ref}}}{k_{\mathrm{B}}T}\right)\right)}$$

  - Molecules: solid blocks mimicking double-stranded DNA molecules with 120 base pairs (40.8nm high, 4 nm wide and a charge of -240q_{e}).
- Material stack: 5nm Al_2O_3/Monolayer MoS_2/27nm SiO_2
- Channel length defined by length of the receptor layer.



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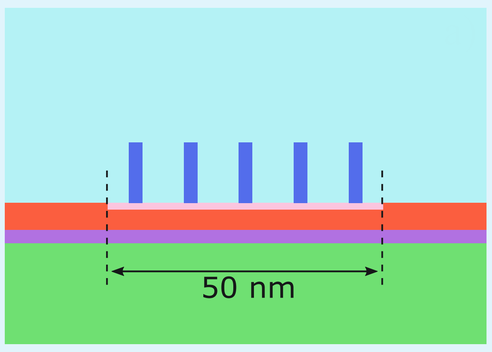
References

[1] S. Mao *et al.*, *Chemical Society Reviews*, vol. 46, no. 22, pp. 6872–6904, 2017. DOI: 10.1039/c6cs00827e

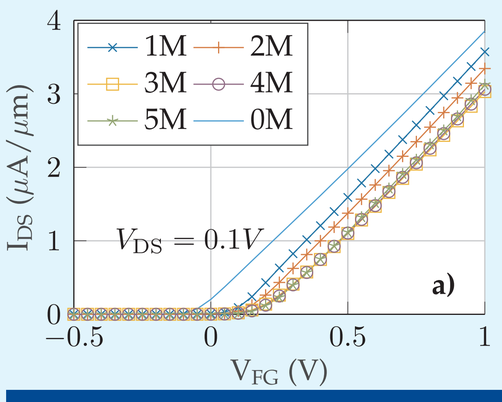
[2] A. Toral-Lopez *et al.*, *Nanoscale Advances*, 2019, **1**, 1077-1085. DOI: 10.1039/c8na00109j

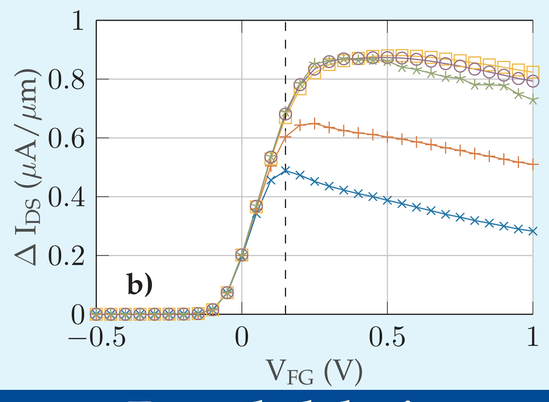
Results

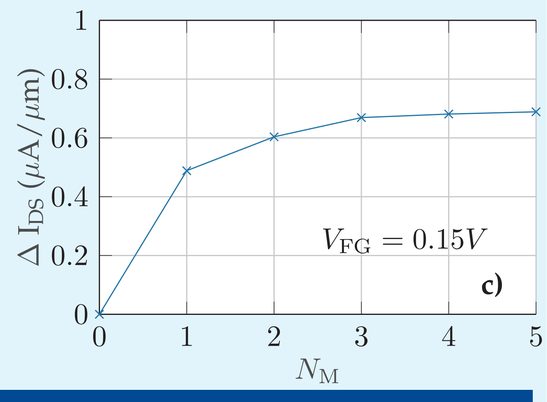
Basic device



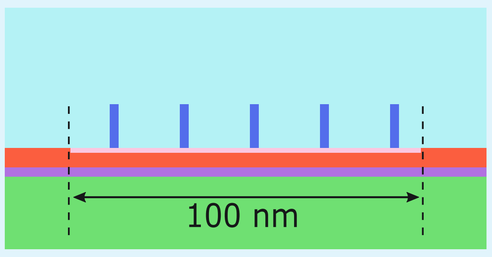
- A 100nm-long MOSFET device is considered with a 50nm long receptor layer placed in the centre of the structure.
- The number of molecules, N_{M}, is increased from 1 to 5, reducing the output current due to their negative charge (Fig.a).
- The sensor output (Fig.b), evaluated as $\Delta I = I_0 - I_{\mathrm{N}}$, shows a saturated trend when $N_{\mathrm{M}} \geq 3$ (Fig.c).



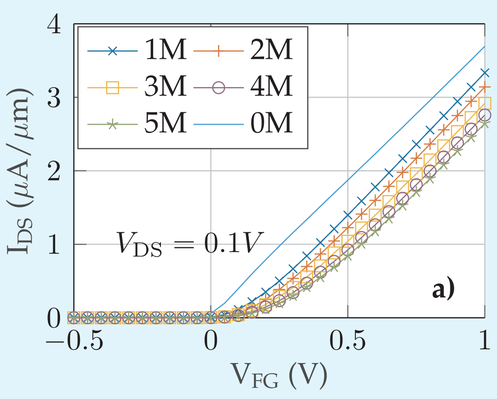


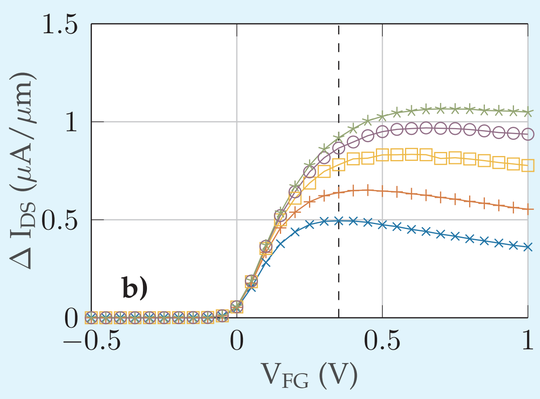


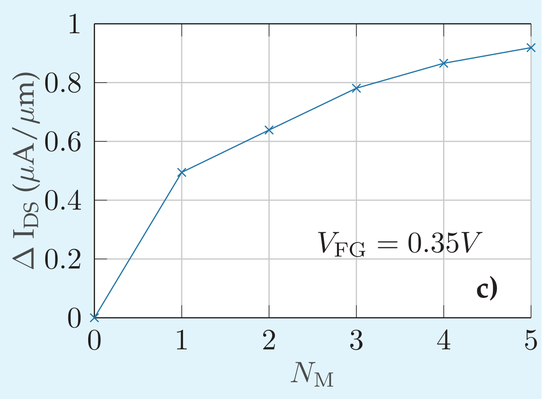
Extended device



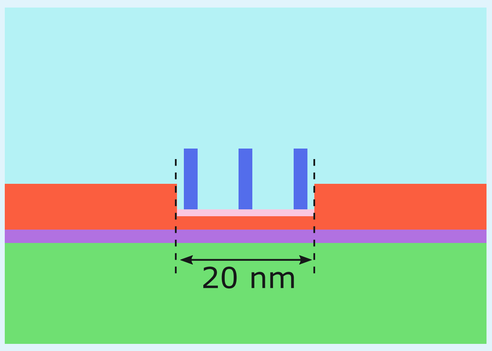
- The lengths of both the semiconductor and the receptor layer are doubled to evaluate the impact of the distance between molecules in the saturation of the sensor output.
- This structure shows an almost monotonous output response. Conclusion: the saturation of the sensor response can be controlled by the receptor layer length.



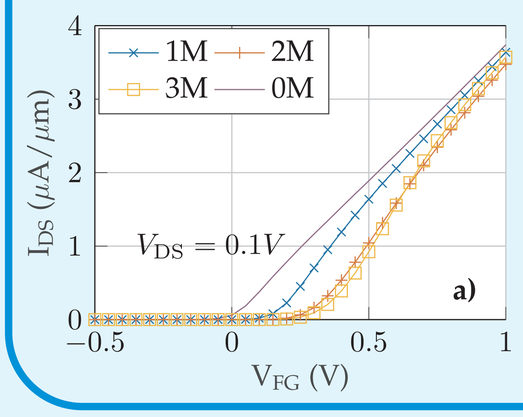


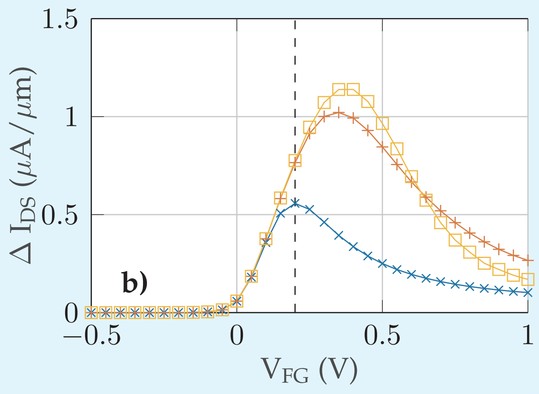


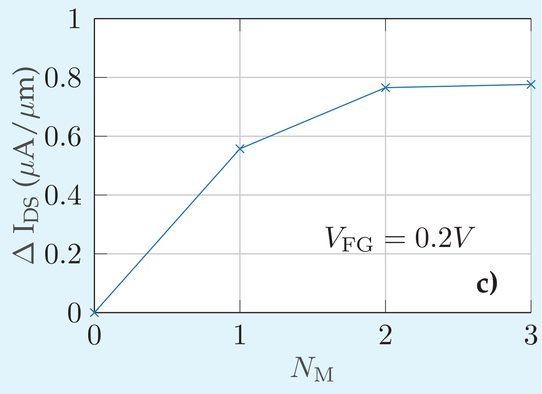
Confined receptors



- A 20nm-long trench is opened in the top oxide to house the receptor layer, thus, confining the molecules and reducing the space between them.
- In this new structure ΔI_{DS} shows a saturated trend for $N_{\mathrm{M}} \geq 2$. This results in a three-state device: $N_{\mathrm{M}} = 0$, $N_{\mathrm{M}} = 1$ and $N_{\mathrm{M}} \geq 2$, which is the tristate expected response of a single molecule sensor.







Conclusions

- A new structure is proposed to detect the single molecule scenario exploiting the modulation of the sensor response saturation using the receptor layer length.
- The size of the trench and the number of slots in the top oxide can be modified to expand the capabilities of BioFETs.