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How can we simulate the detection of nitroaromatic contaminants by graphene-based sensors?

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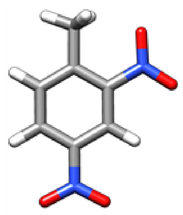
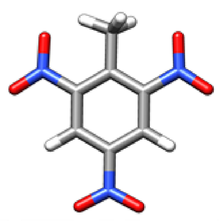
NACs contaminants:

- High contamination of ground and water
- Toxic
- Not biodegradable
- Employed in the production of dyes and drugs or as explosives



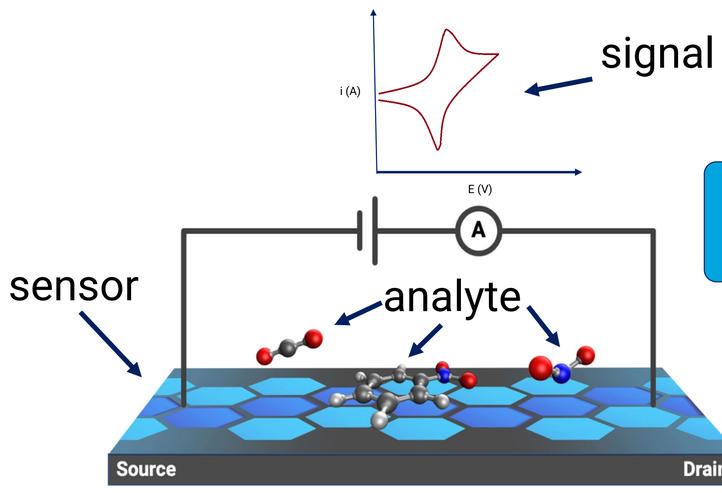
2,4-dinitrotoluene (DNT)

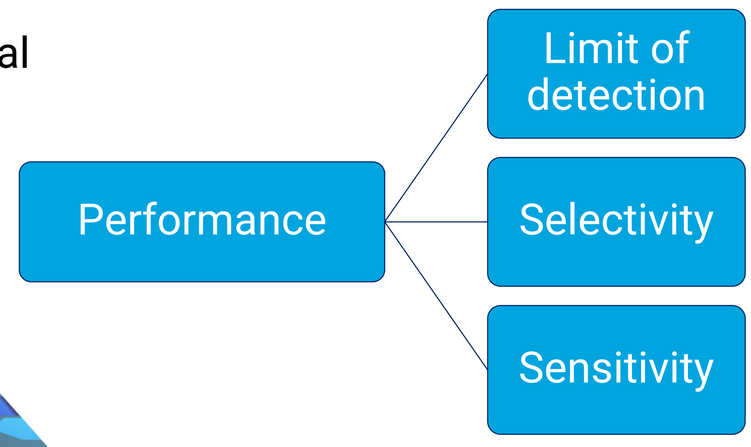


2,4,6-trinitrotoluene (TNT)

Electrochemical graphene-based sensors:

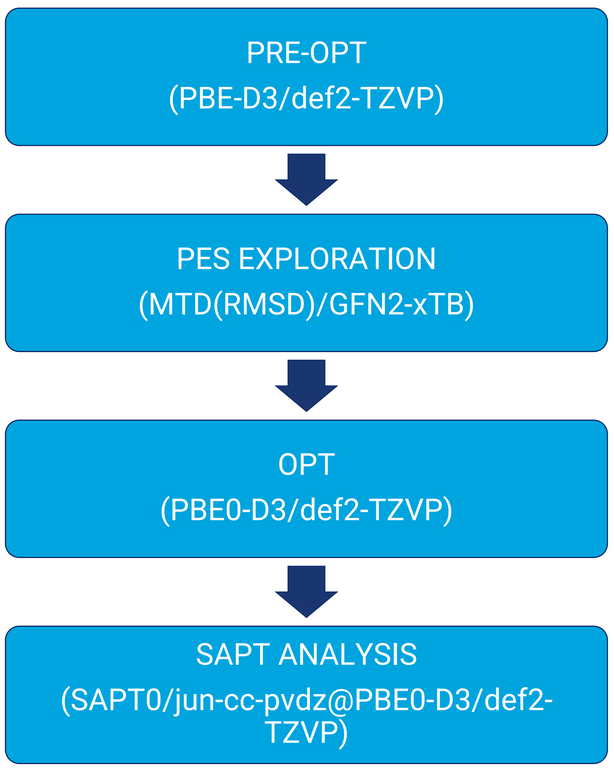
They measure changes in the electric properties of the graphene-based sensor, derived by a redox reaction or physisorption.



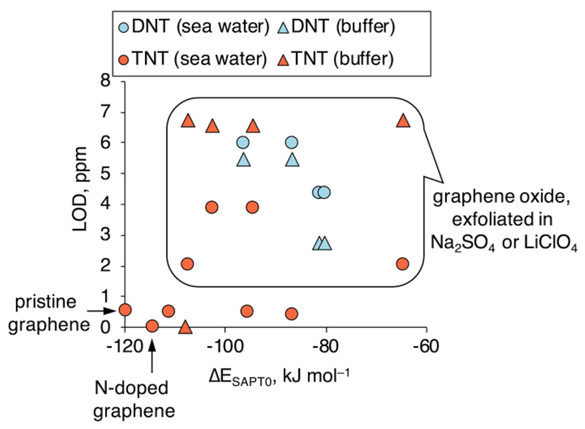


The stronger the **analyte-sensor interaction**, the better the detection **performance**.

Methods:

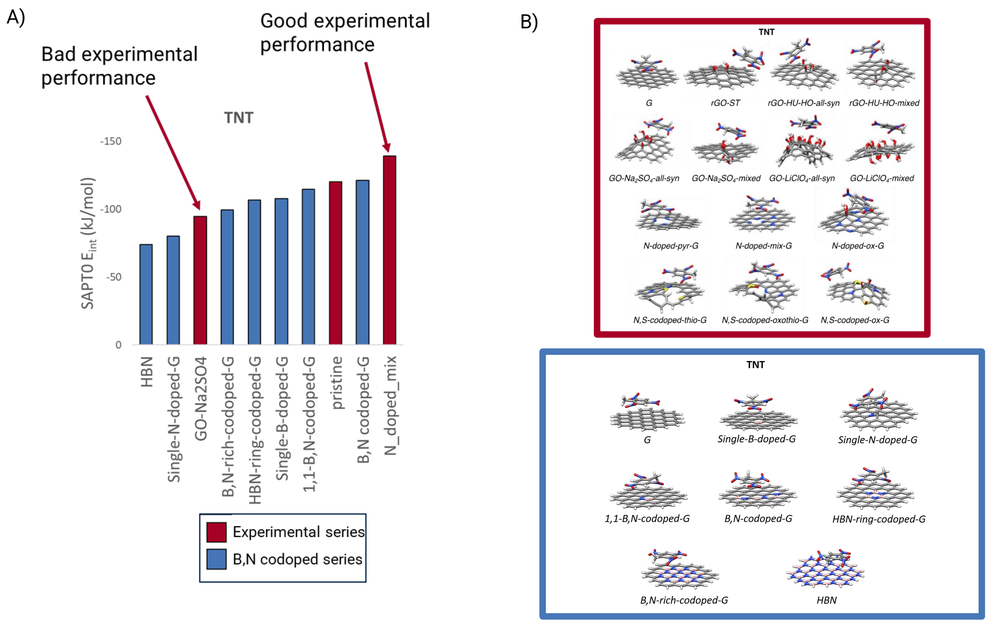


Results:



Experimentally measured limits of detection of DNT and TNT in saline aqueous environments plotted against computed SAPT0/jun-cc-pVDZ interaction energies in NAC-GBM complexes.

Qualitative agreement between strength of interaction and limit of detection.
We can classify "systems" to predict their limit of detection.



A) Selection of computed SAPT0/jun-cc-pVDZ interaction energies in TNT-GBM complexes. B) Three-dimensional structures of the most stable adsorption geometries of the experimental (red rectangle) and B,N-codoped (blue rectangle) series of TNT-GBM complexes (PBE0-D3/def2-TZVP)

Best performance predicted for GBMs with low level of codoping

Conclusions:

- The strength of the sensor-analyte interactions can be correlated with the limit of detection, allowing to predict the behaviour of new graphene-based materials for sensing applications.
- More research is needed to increase the realism of the simulation (periodic, solvent..) and to explore the following steps of the detection (redox reaction).

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REFERENCES

1) Piras, A.; Ehlert, C.; Gryn'ova, G. WIREs Comput Mol Sci., e1526 (2021)
2) Ong, B. K.; Poh, H. L.; Chua, C. K.; Pumera, M.; Electroanalysis, 24 (2012) 2085.
3) Piras, A.; Gryn'ova, G., 10.26434/chemrxiv.14364800.v2 (2021).

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