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The law of attraction:
computational insights into the role of non-covalent interactions in graphene-based sensing

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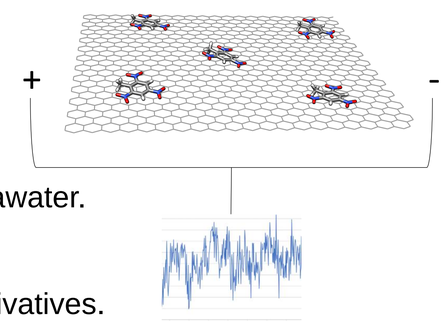
NACs contaminants:
Nitro-aromatic compounds (NACs) like TNT and DNT are dangerous pollutants, contaminating ground and water. They are used in industry in the production of drugs, dyes but also explosives. Their bioaccumulation can lead to liver and blood pathologies.

2,4-dinitrotoluene (DNT) 2,4,6-trinitrotoluene (TNT)

Graphene-based sensors:
Graphene-based sensors electrochemical are:
- Cheap;
- Highly tunable;
- Good to great performances.
- Can be used to detect dangerous contaminants in seawater.

But:
- Difficult to compare the performances for different derivatives.

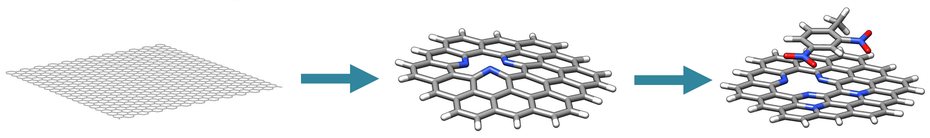


How important are non-covalent interactions in the detection of environmental pollutants by graphene-bases sensors?

Our approach

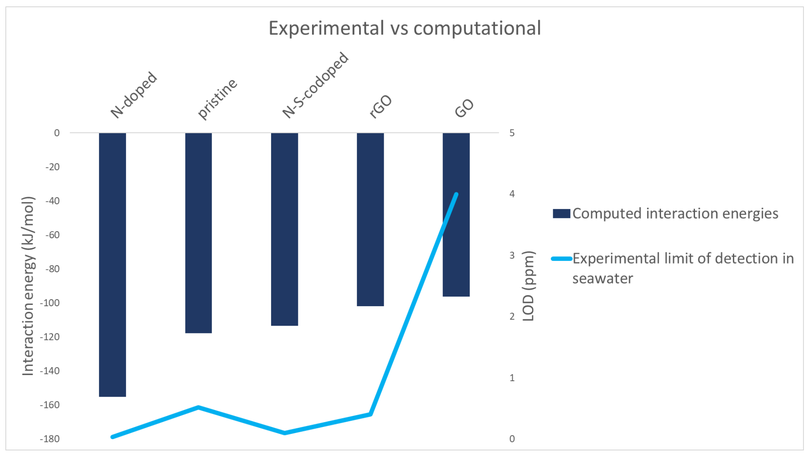
ab initio study on the non-covalent interactions (NCIs) between sensor and analyte → Nature / Strength → NCIs between the graphene-based sensors and the NACs → Detection performance → rational design of graphene-based sensors for NACs contaminants

Key challenge:
Find reliable geometries for NACs on GBMs



Methods:
1. PRE-OPT (PBE/def2-TZVP)
2. PES EXPLORATION (MTD(RMSD)/GFN2-xTB)
3. OPT (PBE0-D3/def2-TZVP)
4. NCIs ANALYSIS (SAPT0@PBE0-D3/def2-TZVP)

Key findings so far:



There is a relationship between the strength of the interaction energy and the experimental detection performances.

Conclusions:
- A computational protocol has been developed to study the interactions between aromatic molecules and different graphene derivatives, employed as electrochemical sensors.
- The strength and nature of these interactions can be correlated with the detection performances (limit of detection in particular).
- The interaction is driven by dispersion, so highly aromatic graphene derivatives, such as N-doped graphene, are more effective than graphene oxide.

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REFERENCES

1) Anichini, C. *et al. Chem. Soc. Rev.* **2018**, 47 (13), 4860–4908;
2) Ong, B. K. *et al. Electroanalysis* **2012**, 24 (11), 2085–2093.
3) Zhang, R *et al. Carbon* **2018**, 126, 328-337.

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