



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



Anna Piras, Christopher Ehlert & Ganna Gryn'ova

Heidelberg Institute for Theoretical Studies (HITS gGmbH), Schloss-Wolfsbrunnenweg 35, 69118 Heidelberg, Germany

Interdisciplinary Center for Scientific Computing (IWR) Heidelberg University, Heidelberg, Germany

NACs contaminants:

- High contamination of ground and water
- Toxic
- Not biodegradable

2,4-dinitrotoluene (DNT)

• Employed in the production of dyes and drugs or as explosives

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.

A)



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





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)

(SAPT0/jun-cc-pvdz@PBE0-D3/def2-TZVP)

Conclusions:

limit of detection. We can classify "systems" to predict their limit of detection.

Best performance predicted for GBMs with low level of codoping

- 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).

CONTACT PERSON Anna Piras anna.piras@h-its.org

MannaPiras19

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