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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
anna.piras@h-its.org

The number of applications of graphene-based materials is quickly increasing. Their high surface-to-volume ratio, electrical and mechanical properties, and number of possible chemical modifications allow producing efficient electrochemical sensors. Computational chemistry is indispensable in clarifying the sensing mechanism and the key factors influencing it [1]. We focus on the detection of two representative dangerous and pervasive nitroaromatic contaminants (NACs), tri-nitro-toluene (TNT) and di-nitro-toluene (DNT). Different graphene-based electrochemical sensors have been developed to detect NACs in water samples [2]. We first studied the role of the analyte's physisorption on the surface with respect to the sensor performance, establishing a qualitative correlation between the strength of adsorption and the experimental limit of detection (LOD), as well demonstrating the definitive effect of physisorption on the sensor's selectivity [3]. These findings were then applied to the design of new potentially high-performance sensor materials based on B,N co-doped graphene derivatives, which displayed good analytical performance at a low level of co-doping. We then proceeded to investigate the electrochemical reduction of the NACs on the sensor surface. Our findings provide key guidelines for designing new and better detection systems.

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., submitted (2021).

Figures

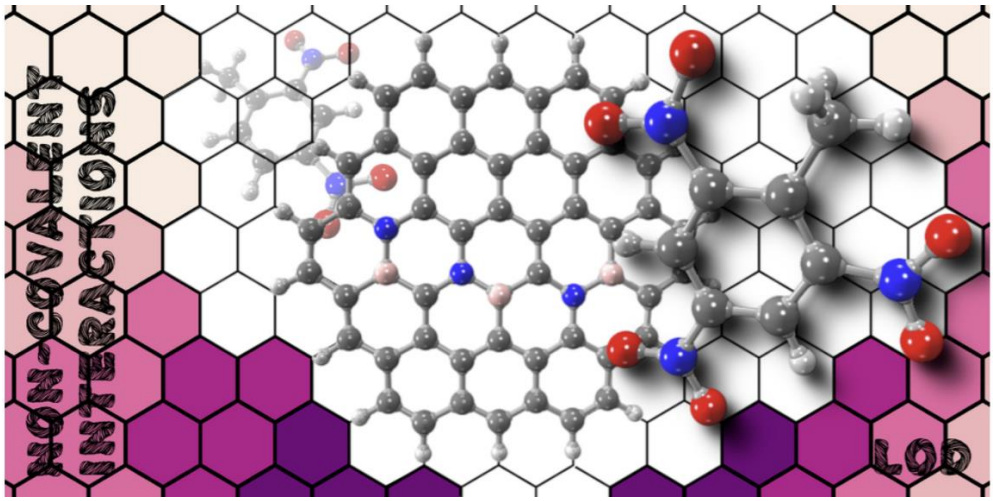

Figure 1: The relationship between in silico estimated non-covalent interactions and the experimental performance is explored for the detection of nitro-aromatic contaminants with graphene-based sensors.