Theoretical study to understand the physicochemical processes of gas analyte interactions with functionalized materials

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New wearable gas sensors based on functionalized 2D materials, notably on carbon nanotube, graphene, or MoS_2, have been developed to detect sub-ppm-level NO_2, NO, CO, or CO_2 pollutants, in a highly selective manner, in urban environments. This theoretical study targets to give an overview of the adsorption processes and electronic properties of the resulting gas sensor at the molecular scale.
First, functionalized material surfaces by physisorption macromolecules, such as metal porphyrins or metal phthalocyanines, are modelled with a procedure based on the density functional theory (DFT) with inclusion of long-distance van der Waals interactions [1, 2, 3]. The effect of the adsorption of these functionalizing molecules on the electronic structure of the material surface is studied. Then, we focus on the interaction of gas molecules (NO_2, NO, CO …) with the nanomaterials before and after functionalization. This modeling study is based on the use of standard codes (GAUSSIAN for macrocyclic and gas molecules [4], and CRYSTAL [5] for surfaces of functionalized materials with adsorbed gas) and compared to experimental results.
Such modelling approach brings insights to better understand the processes occurring at the gas/functionalized material layer interface, particularly concerning the charge transfers between the different elements of the sensor, (gas + functionalizing molecules + material), and the type of doping of the material after functionalization and after adsorption of gases.
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KEYWORDS: Functionalization, 2D materials, gas surface interaction, DFT.

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