Density functional theory calculations of graphene-based humidity and carbon dioxide sensors: effect of silica and sapphire substrates

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Abstract
In this work we investigate the possibility of using graphene as a carbon dioxide and humidity sensor. Carbon dioxide and water adsorbates are modeled on top of the surface of a graphene sheet, which themselves lie on one of two types of silica substrates or sapphire substrate. We evaluate the changes in the electronic and structural properties of the graphene sheet in the presence of the described adsorbates as well as the accompanying substrate. We perform computations based on density functional theory (DFT), that allows fast, accurate and efficient investigations. In particular, we focus our attention on investigating the effects of defects in the substrate and how it influences the properties of the graphene sheet. The defects of the substrate contribute with impurity bands leading to doping effects on the graphene sheet, which in turn together with the presence of the adsorbates result in changes of the electronic charge distribution in the system.

References