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

Karim Elgammal [1, 2], Håkan W. Hugosson [1], Anderson D. Smith [3], Mikael Råsander [4], Lars Bergqvist [1, 2], Anna Delin [1, 2, 5]

[1]*Department of Materials and Nano Physics, School of Information and Communication Technology, KTH Royal Institute of Technology, Electrum 229, SE-16440 Kista, Sweden,*
[2]*SeRC (Swedish e-Science Research Center), KTH Royal Institute of Technology, SE-10044 Stockholm, Sweden,*
[3]*Department of Integrated Devices and Circuits, School of Information and Communication Technology, KTH Royal Institute of Technology, Electrum 229, SE-16440 Kista, Sweden,*
[4]*Department of Materials, Imperial College London, SW7 2AZ, London, United Kingdom,*
[5]*Department of Physics and Astronomy, Materials Theory Division, Uppsala University, Box 516, SE-75120 Uppsala, Sweden*
elgammal@kth.se

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
[1] Anderson David Smith, Karim Elgammal, Frank Niklaus, Anna Delin, Andreas Fischer, Sam Vaziri, Fredrik Forsberg, Mikael Råsander, Håkan W. Hugosson, Lars Bergqvist, Stephan Schröder, Kataria Satender, Mikael Östling and Max Lemme, Resistive Graphene Humidity Sensors with Rapid and Direct Electrical Readout, Nanoscale, 45, 19099-19109, (2015) http://doi.org/10.1039/C5NR06038A}{http://doi.org/10.1039/C5NR06038A.

[2] Karim Elgammal, Håkan W. Hugosson, Anderson D. Smith, Mikael Råsander, Lars Bergqvist, Anna Delin, Density functional theory calculations of graphene-based humidity and carbon dioxide sensors: effect of silica and sapphire substrates, Draft phase.