

Oxygen at Graphene/Cu(111) and Graphene/TiO₂(101) Interfaces: a Van der Waals DFT Study

Cristiana Di Valentin¹, Lara Ferrighi¹, Gianluca Fazio¹

¹*Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, via Cozzi 55, Milano, 2015 ITALY.*

email: cristiana.divalentin@mater.unimib.it

The observation of an enhanced chemical reactivity at graphene/support interfaces is currently a hot topic of research and it is rationalized as the consequence of the two-dimensional confinement effect. In this context we have investigated, by means of density functional theory (DFT) calculations and the periodic supercell approach, the oxygen reactivity at the interface of pristine and B-doped graphene with both crystalline Cu (111) [1,2] and anatase TiO₂ (101) surfaces [3]. In this talk we will present an overview of our results. We will show that, to properly describe interface distances, adhesion energies, electronic properties and charge transfer effects, the use of Van der Waals corrected methods is mandatory. In the case of TiO₂, some portion of exact exchange, as in the hybrid functional approaches, is also required, to avoid spurious effects deriving from an underestimated band gap value for the semiconducting oxide. The presence of oxygen at the interface is found to enhance the adhesion energy of pure and doped graphene with both substrates. The role of the dopant is to increase the interaction with the oxygen atoms. All these observations indicate a positive effect of oxygen confinement at a graphene/substrate interface in terms of improved reactivity, interfacial charge transfer and electronic states hybridization.

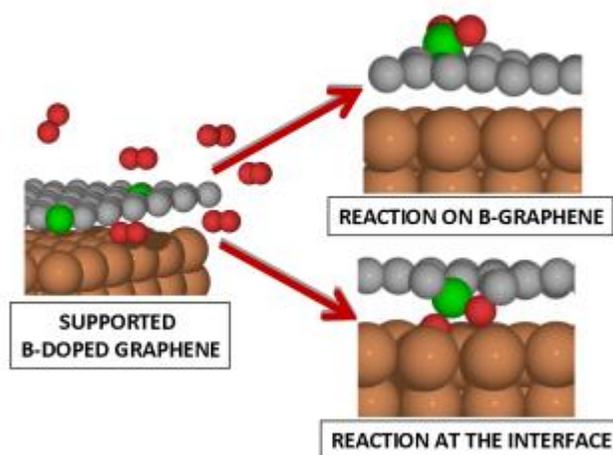


Figure caption: Schematic representation of oxygen reactivity at the doped graphene/support interface.

References:

- [1] L. Ferrighi, M.I. Trioni, C. Di Valentin *J. Phys. Chem. C* **119**, 6056-6064 (2015).
- [2] L. Ferrighi, C. Di Valentin *Surf. Sci.* **634**, 68-75 (2015).
- [3] L. Ferrighi, G. Fazio, C. Di Valentin, under review.