

Chemistry makes graphene interfaces great again : a first-principles investigation

M.-L. Bocquet

*PASTEUR, Département de chimie, Ecole Normale Supérieure, PSL University, Sorbonne
Université, CNRS, 75005 Paris, France*
marie-laure.bocquet@ens.fr

Graphene is an attractive candidate for carbon-based electronic devices. However the absence of band gap is a major hindrance for this promising application. There is a need to develop facile routes for engineering the band gap via covalent functionalizations. The challenge resides in the fact that graphene is assumed to be chemically inert [1] except under harsh conditions.

In this talk I will show how graphene can be properly activated to react under mild and sustainable conditions. First I will describe a feasible route of cycloaddition on a specific UHV graphene/metal interface and explain the desired characteristics of the underlying metal. The interface reactivity has some resemblances with the favorable metallic clusters adsorption studied earlier. [2] Such cycloaddition process has been realized at the single-molecule level by STM-induced chemistry on low-coverage iron phthalocyanine (FePc) molecules adsorbed on graphene on Ir. [3]

Second I will discuss the chemical reactivity of graphene in a water media. Recent nanofluidic experiments have demonstrated the significant charging capacity of carbon [4] and boron nitride [5] nanotubes of diameters ranging from 7nm to 70 nm in alkaline water for promising applications in blue energy. Static DFT calculations in vacuum and implicit water contradict the charging via chemisorption of hydroxide ions on single layer graphene. [6]. However our recent AIMD simulations with explicit water solvent permit to reconcile the atomistic quantum simulations with the experiments.

References:

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