Ab-initio study of electronic proprieties of two-dimensional materials

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Abstract :

During several years, it was believed that the existence of free-standing two dimensional (2D) crystals was impossible. The experimental accomplishment of synthesizing two-dimensional isolated sheets of graphene has led to the emergence of a truly new physics. However, in spite of the discovery of graphene and of its extraordinary electronic properties, the lack of an intrinsic band gap in graphene is a major obstacle for certain applications. To overcome the disadvantages, many efforts have been attempted, such as the chemical functionalization of graphene or by exploring other graphene-like such as ultrathin group metal chalcogenides.

We have studied graphene chemically functionalized by various molecules like the hydroxyl group (-OH), the nitrile group (-CN) or the methyl group (-CH3), using density functional theory (DFT). For each type of molecule, we have studied two possible systems: the first one is a single molecule on a supercell of graphene, while the second one is graphene fully covered by molecules. We found, in particular that the systems are metallic when a single group is attached to the sheet of graphene and a large bandgap is obtained at full coverage. Our GW calculations give a direct or indirect band gaps ranging between 5.5 to 6.5 eV.

We have also investigated the electronic properties of the indium and gallium chalcogenide bilayers. The GW approximation was used to calculate the bandgap and the correction TS-HI was used to describe correctly Van der Waals interactions between layers as implemented in VASP. We found InSe and GaSe bilayers are indirect-gap semiconductors, with electronic gap of 2 eV and 2.71 eV, respectively. Also, we have shown that due to their particular band alignment, some heterobilayers enable electron-hole separation which is of interest for solar cell applications.

Contribution: Invited