Density-functional-theory calculations on graphene and related materials

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Abstract

Some recent results of first-principles calculations of graphene-related materials will be reviewed. The calculations are based on density-functional theory (DFT) using the Siesta method. From early calculations of the phonon spectra of graphene and nanotubes [1], to calculations of bilayer graphene nanoribbons [2], the calculations demanded the possibility of efficient simulations with large number of atoms, as implemented in Siesta, which is capable of linear-scaling DFT calculations, i.e. calculations whose cost in CPU and memory scale linearly with the number of atoms in the unit cell, as opposed to the conventional cubic scaling of canonical DFT. In many situations related to graphene and derivatives, Van der Waals interactions are crucial. The very efficient recent implementation [3] of the fully first-principles, fully non-local density functional proposed in 2004 [4] and its variants [5-7] have allowed more accurate simulations of bilayer graphene, both for the mentioned ribbons [2] and for the study of divacancy defects in bilayer graphene motivated by electron microscopy findings [8]. Similar large scale calculations have also allowed the supporting of results obtained more formally for insulating compounds in the graphene-like honeycomb structure and their heterostructures [9]. Effective fractional charges of e/3 are found as fundamental charge in the polarization discontinuity at the interface between two of such insulators, the origin of such well-defined charges being in many ways analogous to what found in symmetry protected topological phases (the two insulators at each side of the interface corresponding to different symmetry-defined values of the Berry-phase associated to polarization). This is analogous to the physics behind [10] the two-dimensional electron gases appearing at interfaces between some perovskite materials [11], and one-dimensional gases proposed at steps of such interfaces [12]. In graphenic insulators, one-dimensional electron gases should also appear, which have a high probability of being half metallic (metallic for one spin direction only) [9].

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