Theoretical study of silicene and germanene

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Graphene is currently a material of considerable scientific and technological interest [1,2]. However, the integration of graphene in current Si-based nanotechnologies is still facing important challenges. Recently, the possible growth of silicene, the silicon counterpart of graphene, on Ag(111) [3] and ZrB_2 [4] substrates has been reported. The electronic properties of silicene and germanene (2D hexagonal Ge) have also been studied theoretically [5-7], both materials being predicted to be gapless semiconductors with linear energy dispersion relations near the K points, like graphene. If one could grow silicene and/or germanene, their integration into nanoelectronic devices would be most likely much favored over their carbon-based counterpart.

Theoretical insights are reported here regarding the structural, vibrational and electronic properties of silicene and germanene grown on various substrates, using density functional theory (DFT). The electronic properties of these 2D materials are found to be strongly influenced by their interaction with the underlying substrate.

We first studied the interaction of silicene with Ag(111) surfaces. Different possible structures of silicene on Ag(111) have been identified, using scanning tunneling microscopy analysis [8,9]. We focus here on the (4x4) silicene/(111)Ag structure, shown on Fig. 1 (a). Due to the substrate-induced symmetry breaking in the silicene layer (non equivalent number of Si atoms on top and bottom positions), the silicene layer is semiconducting, with an energy gap of about 0.3 eV. However, the interaction with the underlying Ag(111) substrate leads to an overall metallic system, as shown in Fig. 1 (b), with a large spread in the projected Si electronic density of states (PDOS), due to the distribution of Si-Si bong lengths, bond angles and buckling distances in the silicene layer.

We next investigated the interaction between silicene or germanene with (0001) ZnS or (0001) ZnSe (semiconducting) surfaces. These wurtzite (hexagonal) materials were chosen based on the nearly perfect matching of their lattice parameters with the one of silicene or germanene [10]. Very interestingly, silicene/(0001)ZnS and germanene/(0001)ZnSe interfaces are predicted to be semiconducting, with computed (indirect) energy band gaps of about 0.7 and 0.4 eV, respectively, the energy gap opening being related to the charge transfer between the Si (Ge) $3p_z$ ($4p_z$) orbitals with the Zn 4s and S 3p or Se 4p orbitals. Most importantly, we found that the nature (direct or indirect) and amplitude of the energy band gap can be controlled by an external electric field (applied perpendicular to the silicene or germanene layer), as illustrated in Fig. 2 for the silicene/(0001) ZnS system.

In summary, silicene and germanene appear as fascinating 2D materials, their electronic properties being largely determined by their interaction with the underlying substrate. The predicted electric field tunable energy band gap of silicene and germanene is very promising for their potential use in nanoelectronic devices.

References
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(a)

(b)
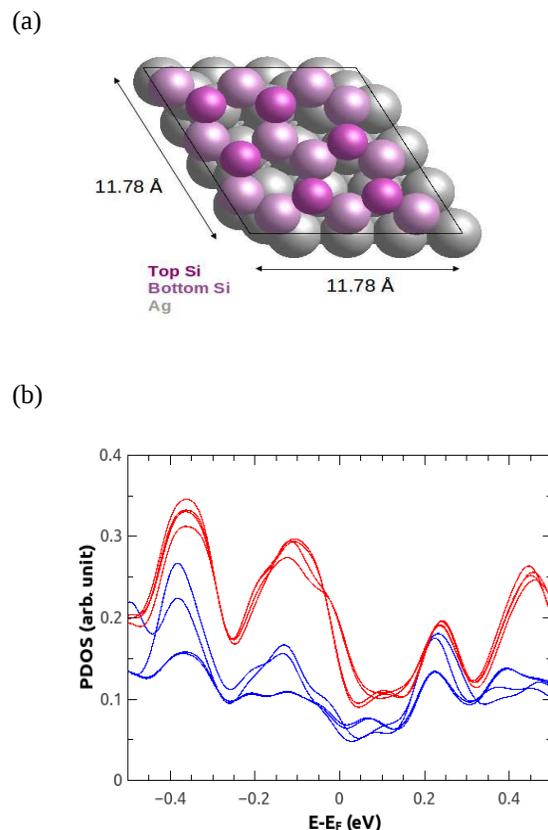
Fig. 1. (a) Top view of the (4x4) silicene/(111)Ag structure, obtained after energy relaxation. The average distance between the top Si (bottom Si) atoms and the Ag surface is 2.93 Å and 2.18 Å, respectively. (b) Projected density of states of the Si atoms. Red and blue lines correspond to the contribution of top and bottom Si atoms, respectively.
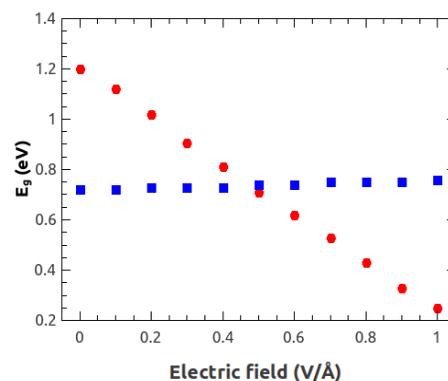
Fig. 2. Computed direct (red circles) and indirect (blue squares) energy band gaps of the silicene/(0001) ZnS interface model, as a function of the applied electric field.