Interaction of germanene with (0001)ZnSe surfaces: A theoretical study

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Graphene is currently a material of considerable interest, both scientifically and technologically [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) [3,4] and ZrB_2 [5] substrates has been reported. The electronic properties of silicene and germanene (2D hexagonal Ge) have also been studied theoretically [6,7], both materials being predicted to be gapless semiconductors with Dirac cones near the K points of the hexagonal Brillouin zone, like graphene. If one could grow silicene or germanene, most preferably on non-metallic substrates, their integration into nanoelectronic devices would be most likely favored over their carbon-based counterpart.

Theoretical insights are reported here regarding the interaction of germanene with (0001)ZnSe surfaces, using density functional theory; ZnSe is a wurtzite (hexagonal) material with in-plane lattice parameters very close to the ones predicted for germanene. We first studied the interaction of germanene on polar (0001)ZnSe surfaces. The most stable structure is shown in Fig.1, corresponding to the formation of a buckled germanene layer on ZnSe. The system is predicted to be metallic, as revealed by the energy band structure shown in Fig.2. The metallic character of this system is due to the pinning of the Fermi level by Se surface states.

We next studied the interaction of germanene with a non-polar reconstructed (0001)ZnSe surface; this surface is predicted to be more energetically stable for thin ZnSe layers (up to about 6 nm) than the polar one, in analogy with ZnS [8]; top and side views of the most energetically stable germanene/(0001)ZnSe interface is shown in Fig. 3. Very interestingly, this system is predicted to be semiconducting, with a computed (indirect) energy band gap of about 0.45 eV, as shown in Fig. 4. The energy gap opening is induced by the charge transfer between the Ge $4p_z$ orbitals with the Zn 4s and 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 germanene layer, as illustrated in Fig. 4. A semiconductor to metal transition is predicted to occur at about 0.6V/Å; this electric field-driven electronic transition appears very promising for the potential use of germanene in field effect devices.

References

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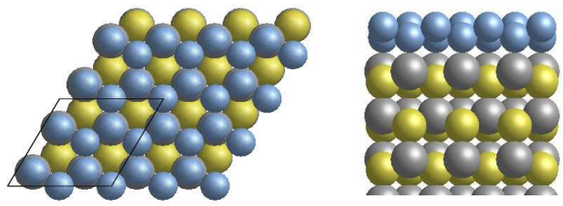

Fig.1. Top (left) and side (right) views of the germanene/polar (0001)ZnSe interface model. Blue, yellow and gray spheres are Ge, Se and Zn atoms, respectively.

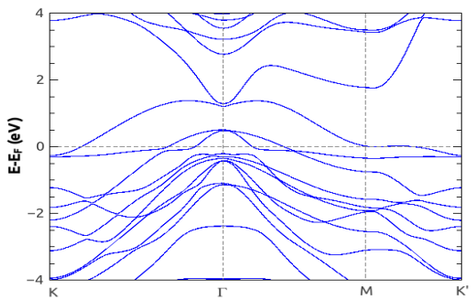

Fig.2. Computed energy band structure of the germanene/ polar (0001)ZnSe interface model. The reference (zero) energy level corresponds to the Fermi level.

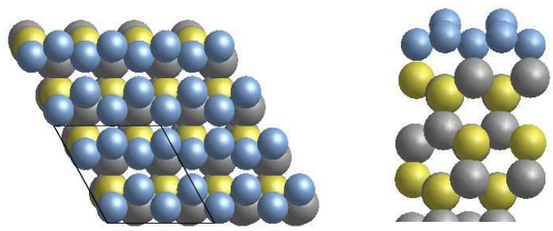

Fig.3. Top (left) and side (right) views of the germanene/non-polar (0001)ZnSe interface model. Blue, yellow and gray spheres are Ge, Se and Zn atoms, respectively.

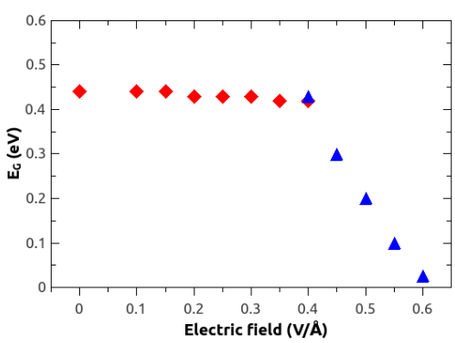

Fig.4. Computed indirect (red diamonds) and direct (blue triangles) energy band gaps of the germanene/non-polar (0001) ZnSe interface model, as a function of the applied electric field.