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Stability of freestanding silicene, silicene nanoribbons and other honeycomb structures

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Abstract:

Since the synthesis of the two-dimensional honeycomb structure of carbon atoms, graphene, the scientific community has revealed many exotic properties owing to the low-dimensionality and structural symmetry of this material. The similarities between carbon and silicon atoms raise the question of transferring these properties to the well-established silicon technology by building the silicon analog of graphene, namely silicene. We have investigated the possibility of the freestanding silicene structure using the stringiest theoretical test involving the calculation of the phonon modes.

Our first-principles calculations of structure optimization, phonon modes, and finite temperature molecular dynamics predict that silicon and germanium can have stable, two-dimensional, honeycomb structures. Unlike graphene, silicene structure is not stable in planar structure, but it is stabilized through buckling (puckering), while preserving the honeycomb symmetry. Similar to graphene, these puckered structures are ambipolar and their charge carriers can behave like a massless Dirac fermion due to their π and π^* bands which are crossed linearly at the Fermi level.

We also present a first-principles study of bare and hydrogen passivated armchair nanoribbons of the puckered single layer honeycomb structures of silicon and germanium. Our study includes optimization of atomic structure, stability analysis based on the calculation of phonon dispersions, electronic structure, and the variation in band gap with the width of the ribbon. The band gaps of silicon and germanium nanoribbons exhibit family behavior similar to those of graphene nanoribbons. Periodic modulation of the nanoribbon width results in a superlattice structure, which can act as a multiple quantum well. Specific electronic states are confined in these wells. Confinement trends are qualitatively explained by including the effects of the interface. In order to investigate wide and long superlattice structures we also performed empirical tight-binding calculations with parameters determined from ab initio calculations.

Finally, we will present our study on monolayer honeycomb structures of group-IV, III-V and transition metal dichalcogenides.