Abstract Submitted
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Single and Few Layer Silicene: Structural, Electronic and Transport Properties[1] J DAVID CAREY, NATHANAEL ROOME, University of Surrey — Single layer silicene has weaker π bonding that graphene resulting in buckling of the Si atoms in different sub-lattices. Despite the loss of planarity, a linear band-structure emerges where we find a Fermi velocity of about 5.3 x 10^5 m/s. Determination of the phonon dispersion characteristics reveals a Γ point optical phonon with an energy of 69 meV and a K point optical phonon with an energy of 62 meV. In graphene these phonons play important role in scattering electrons, and in Raman spectroscopy, but have larger energies of 194 and 166 meV, respectively. The lower phonon energies in silicene, arising from the higher atomic masses, would be expected to scatter carriers efficiently and limit carrier mobility. We have calculated, however, that the electron-optical phonon coupling matrix elements are about a factor of 25 times smaller than in graphene and this important result will help with the further development of silicene based devices due to reduced phonon scattering. The two stable stacking configurations of bilayer silicene, AA and AB, now have to account of the position of the atomic buckling in the two layers, leading to four possible atomic configurations with the buckling between the layers being in- or out-of-phase with each other. We find that in contrast to graphene, the two stable configurations are based on AA type stacking being about 70 meV per atom more stable than AB stacking. The potential for elemental layered materials beyond graphene for device applications will also be discussed.

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