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Electronic and vibrational properties of group IV 2D materials: Planar and buckled forms of graphene, silicene and germanene[1] DAVID CAREY, NATHANAEL ROOME, University of Surrey — We report the ab initio electronic band structure and vibrational properties of 2D group IV elemental materials. Band structure calculations of planar graphene reveal a linear dispersion relation around the Dirac point with Fermi velocities of 8.0, 5.2 and 5.6 x 10^5 m/s, respectively. The behaviour of the unoccupied σ^* mode, normally ignored in planar graphene, is shown to be vary significantly with energy and cross the Fermi level in germanene. Analysis of the vibrational modes indicates that the E_{2g} mode at the zone centre (Γ point) appears at 1566, 604 and 366 cm^{-1}, respectively. Two types of buckling are shown to be present in silicene and germanene and linear dispersion is found in the low buckling configurations of both silicene and germanene. The band structure of silicene and germanene in the high buckling arrangement is shown to be much more complicated with a breakdown of the Dirac cone behaviour. The stability of the different forms of free standing layers is explored and the contribution of the different phonon modes to material stability is discussed. Electron-phonon coupling matrix elements are also calculated.

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