

Abstract Submitted
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Lattice Stacking Interactions: Comparisons between bilayer graphene and silicene DAVID CAREY, NATHANAEL ROOME, Univ of Surrey — The stacking arrangement of atoms in elemental 2D materials, such as graphene and silicene, plays a crucial role in determining their structural, electronic and vibrational properties. The weaker π bonding in silicene results in atomic buckling, and previously we have found linear band dispersion in a low atom buckling geometry with a Fermi velocity about $2/3$ that of graphene and electron-phonon matrix elements are about a factor of 25 times smaller than in graphene [1]. Here we investigate the properties of different stacking configurations of bilayer silicene with those of bilayer graphene (BLG). In the case of BLG there are two stable configurations AA and AB stacking, with no atomic buckling present. In the case of bilayer silicene the presence of buckling and the different stacking arrangements results in a range of stable configurations. We calculate the frequencies of the IR and Raman active modes as a means to identify the different bonding and stacking configurations. This approach of fingerprint identification is applicable to other elemental layered materials.

[1] Beyond Graphene: Stable Elemental Monolayers of Silicene and Germanene, Nathanael Roome and J David Carey, ACS Applied Materials & Interfaces, 6, 7743 – 7750 (2014).

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