First-principles study of stable few-layer pentasilicene: Supplemental material

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I. The bilayer silicene h-si1 structure

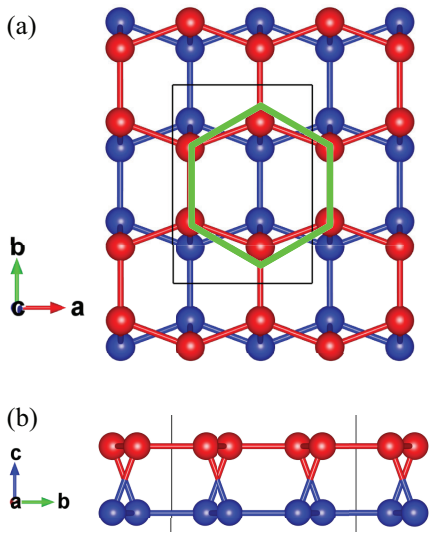

FIG. 1. h-Si1 atomic structure: (a) top view and (b) side view. A perfect hexagonal shape is shown for reference.

We present here some details for the h-Si1 structure of bilayer hexagonal silicene. To the best of our knowledge, this is the first time that such a structure is suggested, although a similar, but different, structure was proposed in Lian and Ni [1] (the intermediate state ISBL). The main difference is that the hexagonal rings in our structure are distorted, as illustrated in Fig. 1, while those in the ISBL structure are perfectly hexagonal. We found that the undistorted ISBL is not stable and will relax to our h-Si1. Additionally, according to the information from Lian and Ni [1], the ISBL has a higher energy than the AA stacked planar hexagonal bilayer silicene, called GSBL in the same paper, while our h-Si1 is 20 meV/atom lower in energy. The h-Si1 has the layer group symmetry cmme (48), which belongs to the orthorhombic crystal system. The length of the **a** and **b** lattice vectors are 4.48 Å and 6.37 Å, respectively. The shorter intralayer bond length is 2.35 Å while the longer one is 2.38 Å . The interlayer bond length is 2.41 Å , which is also the bilayer thickness. The interior angles of the distorted hexagons are 139.4° and 110.4°. The electronic structure is plotted in Fig. 3 and shows that it is a metal. The phonon spectrum of h-Si1 is free of imaginary frequencies (see Fig. 2), which indicates its dynamical stability.

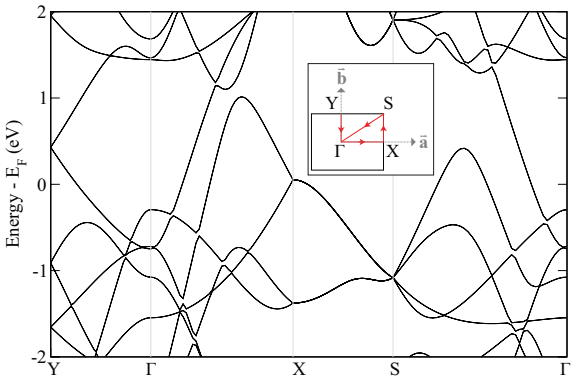

FIG. 2. h-Si1 band structure.

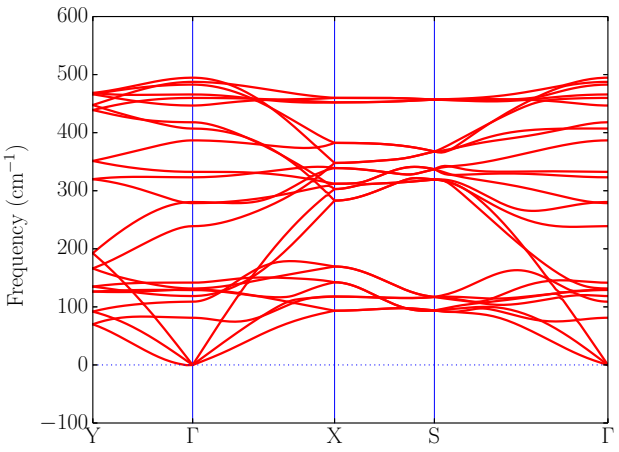

FIG. 3. h-Si1 phonon spectrum.

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[1] C. Lian and J. Ni, AIP Adv. **3**, 052102 (2013).