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Structural and electronic properties of freestanding bilayer silicene YUKI SAKAI, ATSUSHI OSHIYAMA, Department of Applied Physics, The University of Tokyo, Japan — We systematically study the structural and electronic properties of freestanding bilayer silicene within the framework of the density functional theory. Starting from 11 different initial atomic configurations, we find 19 total-energy minimized structures with respect to the in-plane lattice parameter. Six of these 19 structures are found to be thermodynamically stable since they do not possess negative phonon frequency modes in their phonon spectra obtained with the density functional perturbation theory. The interlayer bond lengths of these structures are shorter than 2.5 Å, indicating their covalent-like interlayer interactions. Four of those six structures are described by the 1×1 unit cell (4 silicon atoms in the unit cell) while the other two structures are described by a 2×2 supercell. The structures with a 2×2 supercell have relatively lower total energies than the 1×1 structures. These low-energy structures have local atomic configurations whose bond angles and bond lengths are similar to those of the ideal diamond structure by making protrusion of silicon atoms. The six stable structures are found to exhibit semimetallic or semiconducting electronic properties depending on their stacking geometries.

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