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Unravelling the "Silicene" Growth Mechanism Based on a Seeding Layer Approach[1] WEI JIANG, Univ of Utah, MIAO ZHOU, Chongqing University, FENG LIU, Univ of Utah, FENG LIU TEAM — Unlike *sp*2 graphene, silicon atoms prefer to form *sp*3 hybridized state that gives silicene a buckled geometry. To study how to grow flat silicene, we have investigated the structure and stability of multi-layer "silicene" using *ab initio* methods by introducing a "seeding layer" of silicene on which additional "silicene" layers are grown. The buckling height and the isotropic strain of the seeding layer is shown to play a key in affecting the structure, in particular the flatness of the growing layers. A phase diagram in the parameter space of buckling height and in-plane strain of the seeding layer is constructed to guide the growth of additional "silicene" layer. Furthermore, in contrast to monolayer silicene growth on Ag substrate which exhibits various patterns, only the $\sqrt{3}$-$\sqrt{3}$ pattern is found stable using large supercell calculations. Our calculations suggest that thermodynamically no silicene structures can survive beyond three layers. These results will shed useful lights on experimental growth of flat and low-buckled silicene and help explain existing experimental results.

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