

The atomic and electronic structure of silicene and germanene on substrates

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Abstract:

The growth of the $\sqrt{3}\times\sqrt{3}$ reconstructed silicene on Ag substrate has been frequently observed in experiments while its atomic structure and formation mechanism is poorly understood. Here, by first-principles calculations, we show that the $\sqrt{3}\times\sqrt{3}$ reconstructed silicene is constituted by dumbbell units of Si atoms arranged in a honeycomb pattern. Our model shows excellent agreement with the experimentally reported lattice constant and STM image. We propose a new mechanism for explaining the spontaneous and consequential formation of $\sqrt{3}\times\sqrt{3}$ structures from 3×3 structures on Ag substrate. We show that the $\sqrt{3}\times\sqrt{3}$ reconstruction is mainly determined by the interaction between Si atoms and have weak influence from the Ag substrate. The proposed mechanism opens the path to understanding of multilayer silicene and new bulk allotropes of silicon having dumbbell units. Furthermore, we present the atomic structure of germanene grown on Au substrate. Finally, we show that 2×2 stanene having dumbbell units arranged in a honeycomb structure is a topological insulator and its nanoribbons possess helical edge states.