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$\pi-$conjugtion in Si(111)-($\sqrt{3}$x$\sqrt{3}$) surface: Bamboo hat "silicene"[1] WEI JIANG, Univ of Utah, ZHENG LIU, Tsinghua Univeristy , MIAO ZHOU, Chongqing University, XIAOJUAN NI, FENG LIU, Univ of Utah, FENG LIU TEAM — The newly observed Si(111)-($\sqrt{3}$x$\sqrt{3}$) surface reconstruction that exhibits a 2D-Dirac state has been widely reported, yet its stability was poorly understood. Based on valence bond and conjugation theory, we propose a π-conjugation plus charge-transfer model underlying its structural stability and unique electronic properties. The "bamboo hat" surface geometry facilitates the formation of unusual planar Si-rings with π-conjugation and charge transfer from the rings to upper buckled Si atoms, to lower the surface dangling bond energy. This intriguing mechanism is confirmed by calculating surface energies and surface stress tensors, explaining the observation of the ($\sqrt{3}$x$\sqrt{3}$) surface grown on the Ag substrate rather than the bulk-terminated Si(111)-(2x1) surface. The same mechanism also applies to the metastable ($\sqrt{21}$x$\sqrt{21}$) surface reconstruction observed in recent experiments.

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