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Reversible hydrogenation of silicene JINGLAN QIU, HUIXIA FU, LAN CHEN, KEHUI WU, Institute of Physics, Chinese Academy of Sciences — The hydrogenation of monoatomic silicene sheet on Ag(111) was studied by scanning tunneling microscopy and density functional theory calculations. It was observed that hydrogenation of silicene-4x4 structure at room temperature results in a perfectly ordered γ-4x4 superstructure. A theoretical model, which involves 7 H atoms and rearranged buckling of Si atoms, was proposed and agrees with experiments very well. Unlike silicene-4x4, the hydrogenation of ($\sqrt{}$7x$\sqrt{}$7)silicene/(2$\sqrt{}$3x2$\sqrt{}$3)R30°Ag(111) superstructure at room temperature shows silicene-1x1 structure with $\sqrt{}$7x$\sqrt{}$7 reconstruction Moreover, by annealing to a moderate temperature, about 450 K, dehydrogenation process occurs and the clean silicene surface can be fully recovered. Such reversible hydrogenation suggests that silicene may be a potential candidate as hydrogen storage materials.

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