

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**Ag(111)- $\sqrt{3}\times\sqrt{3}$ -Silicene Versus Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface**<sup>1</sup> HUI LI, State Key Laboratory for Surface Physics, Institute of Physics Chinese Academy of Sciences — Since 2012, silicene has been successfully grown on Ag(111) surface. We have provided reasonable atomic models of  $\sqrt{3}\times\sqrt{3}$  silicene. However, the atomic and electronic structures of  $\sqrt{3}\times\sqrt{3}$  silicene are still heavily debating, especially, it is easily to be confused to the Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface. Here, I give a report of our recent works on silicene. With first-principles calculations combined with STM observations, we studied the structures of multilayer silicene on Ag(111) substrates, which all have  $\sqrt{3}\times\sqrt{3}$  relaxed surfaces, and diamond-like stacking mode. Both calculations and STS show such silicon surface has strong Dirac-cone-like surface state, indicating the multilayer silicene possesses a new kind of silicon surface. The Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface is further compared to epitaxial silicene. It is found that the simulated STM images of both surfaces are similar, there is also strong surface state for Si(111)- $\sqrt{3}\times\sqrt{3}$ -Ag surface. However, the different temperatures for symmetry-breaking phase transitions and different H-adsorption structures can be used for distinguishing such two surfaces.

<sup>1</sup>silicene

Hui Li  
State Key Laboratory for Surface Physics,  
Institute of Physics Chinese Academy of Sciences

Date submitted: 14 Nov 2014

Electronic form version 1.4