Abstract Submitted for the MAR13 Meeting of The American Physical Society

Absence of Dirac Electrons in Silicene on Ag (111) Surfaces ZHI-XIN GUO, SHINNOSUKE FURUYA, JUN-ICHI IWATA, ATSUSHI OSHIYAMA, Department of Applied Physics, The University of Tokyo, Tokyo 113-8656, Japan — We report first-principles calculations that clarify stability and electronic structures of silicene on Ag(111) surfaces. We find that several stable structures exist for silicene /Ag(111), exhibiting a variety of surface morphology. We also find that Dirac electrons are absent near Fermi energy in all the stable structures due to buckling of the Si monolayer and mixing between Si and Ag orbitals. We propose that either BN substrate or hydrogen processing of Si surface is a good candidate to preserve Dirac electrons in silicene.

> Zhi-Xin Guo Department of Applied Physics, The University of Tokyo, Tokyo 113-8656, Japan

Date submitted: 05 Nov 2012

Electronic form version 1.4