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Electronic structures and transport properties of silicene on Ag surface YUN-PENG WANG, HAI-PING CHENG, Physics Department of Physics and the Quantum Theory Project, University of Florida — It has been predicted from first-principle that "silicene", a two-dimensional buckled honeycomb structure of silicon, is thermally stable and has a graphene-like band structure. In experiments, epitaxial silicene were observed to form at hexagonal Ag(111) and $ZrB_2(0001)$ surfaces. However, electronic structure and transport properties related to silicene have not been thoroughly studied. In this work, we have studied band structures of silicene on top of Ag surface using density-functional theory. The effective band structure mapped onto 1×1 unit cell of monolayer silicene on Ag(111) surface could be compared directly with Angle-Resolved Photoemission Spectra (ARPES). We have also studied electronic transport property across monolayer and bilayer silicene sheets using the Non-Equilibrium Green's Function (NEGF) method. The transmission curve shows a maximum at Fermi energy for the monolayer silicene case, but shows a minimum for the bilayer silicene case, which can be explained by their band structures.

Yun-Peng Wang
Physics Department of Physics and the Quantum Theory Project,
University of Florida

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