Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Semiclassical Boltzmann Theory Studies of the Electronic Resistances of Multilayered Silicene Junctions[1] YUNPENG WANG, X.-G. ZHANG, JAMES FRY, HAI-PING CHENG, University of Florida — A layer-by-layer investigation is carried out to understand electron transport across metal-semiconductor-metal junctions. Structures of junctions are optimized using first-principles density functional theory with the generalized gradient approximation. The semiclassical Boltzmann theory of the electronic transport is revisited and applied to multilayer silicene and hexagonal BN based junctions. The calculated resistance is smaller than, but converges to that calculated by the Landauer formula as the thickness of the barrier increases. Our calculation results provide an upper limit on the transmission coefficient per channel, ~ 0.05, below which the Landauer formula is applicable for calculating the resistance. In addition, we find that the resistance of a junction is not determined entirely by the average transmission, but also by the distribution of the transmission over the first Brillouin zone.

[1]This work was supported by the US Department of Energy (DOE), Office of Basic Energy Sciences (BES), under Contract No. DE-FG02-02ER45995. This research used resources of the National Energy Research Scientific Computing (NERSC) Center.

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Date submitted: 14 Nov 2014 Electronic form version 1.4