Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Stability and Electronic Properties of Two-Dimensional Silicene and Germanene on Graphene CHIH-PIAO CHUU, YONGMAO CAI, C.-M. WEI, M.-Y. CHOU, Academia Sinica — Recently, there have been experimental attempts to synthesize silicene, a two-dimensional (2D) graphene-like form of silicon on metal surfaces such as Ag(111) and Ir(0001). The possibility of preparing silicene on ZrB2 thin films grown on silicon wafers has also been reported. This suggests new perspectives for the applications of massless fermions in materials that are compatible with Si-based electronics. It is expected that many of the unique electronic properties of graphene can also be realized in this new 2D system. However, the interaction between the 2D silicon structure and the metal substrate is found to be quite strong, leading to distortion in the adlayer and consequently the disappearance of the Dirac cone. Therefore, finding a suitable substrate that interacts with silicene weakly and preserves the sublattice symmetry is of ultimate importance. We have performed first-principles calculations of silicene and germanene on graphene in order to understand the effect of substrate interaction on the physical properties of these systems. Of particular interest is the induced change in the electronic structure, the modification of the Fermi velocity, the gap opening, the charge doping from the substrate, and the stability of the combined system. The energetics of forming the 2D silicone structure on a substrate is carefully evaluated in comparison with possible three-dimensional cluster structures.

Chih-Piao Chuu
Academia Sinica

Date submitted: 14 Nov 2013 Electronic form version 1.4