Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Topologic connection between a (quasi) 2-D hexagonal and 3-D diamond or wurtzite structure JIANWEI WANG, YONG ZHANG, University of North Carolina at Charlotte — The similarity in the geometrical arrangements of C atoms between the (111) plane of diamond and the basal plane of graphite has long been recognized.[1] Individual (111) monolayers of various IV and III-V compounds have been explored theoretically as candidates for 2-D materials beyond graphene.[2] We further point out the topologic connection between the 2-D hexagonal and 3-D diamond (zinc-blende) or wurtzite structure, namely a buckled 2-D hexagonal structure (e.g., silicene) can be viewed as a partially collapsed 3-D (111) or (0001) monolayer when the monolayer spacing is increased and in the meantime allowing the structure to relax into a (meta)stable configuration. Graphene is one of the special cases the monolayer collapses entirely. Using a density functional theory, we examine this topologic evolution for IV, III-V, and II-VI compounds and calculate the electronic structures for the quasi 2D structures so derived. When large atoms are involved, the weakened π-bond of the monolayer leads to chemical instability. Capping layers can be used to stabilize the material, which then forms an ultra-thin quantum well or superlattice.[3] [1] Li et al., JAP 73, 711(1993).[2] Şahin et al., PRB 80, 155453 (2009). [3] Esaki & Tsu, IBM Res. Develop. 14, 61 (1970).

Jianwei Wang
University of North Carolina at Charlotte

Date submitted: 14 Nov 2013 Electronic form version 1.4