

Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Stabilizing Graphitic Thin Films of Wurtzite Materials by Epitaxial Strain¹ DANGXIN WU, FENG LIU, University of Utah — Recent theoretical and experimental work showed that (0001) ultrathin films of wurtzite materials transform into a stable graphite-like structure if their thickness is reduced to only a few atomic layers. Using first-principles calculations of both freestanding and substrate-supported thin films, we predict that the thickness range of stable graphitic films can be greatly extended by epitaxial tensile strain but reduced by compressive strain. The band gap of the resulting graphitic films can be tuned by strain and film thickness either above or below that of the bulk wurtzite phase. Our prediction suggests a plausible physical mechanism to be explored by future experiments for strain engineering of graphitic films from wurtzite materials with a wide range of potential applications.

¹This work is supported by DOE-BES.

Dangxin Wu
University of Utah

Date submitted: 17 Nov 2010

Electronic form version 1.4