Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Stability and work function of TiC_xN_{1-x} alloy surfaces: Density functional theory calculations[1] HONG ZHU, MARK AINDOW, RAMPI RAMPRASAD, University of Connecticut — Critical factors that control the vacuum work function of the TiC_xN_{1-x} ternary system surfaces were determined using detailed density functional theory calculations. Although the work function of the most stable surfaces does vary with the alloy composition (i.e., $x$value), surface chemistry (i.e., orientation, stoichiometry, and defect density) was found to play the most important role in determining the work function value, far surpassing the impact of alloy composition on the work function. In general, Ti-deficient surfaces display larger work functions. Work function tuning may thus be effectively accomplished by controlling the surface chemistry rather than the composition.

[1]Financial support of this work through a grant from the National Science Foundation (NSF) and computational support through a NSF Teragrid Resource Allocation are gratefully acknowledged.

Hong Zhu
University of Connecticut

Date submitted: 19 Nov 2009 Electronic form version 1.4