Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Wannier-functions disentanglement to determine Schottky barrier heights: application to CNT-metal systems NICHOLAS SINGH-MILLER, NICOLA MARZARI, Massachusetts Institute of Technology — We study Schottky barrier heights in carbon nanotube CNT-metal junctions using pseudopotential plane-wave density functional calculations. We determine the barriers by two methods: first through a line-up of the local electrostatic potentials at the junction with respect to bulk reference systems, and second by directly extracting the band structure of the semiconducting nanotube from the entire manifold of the electronic states of the CNT-metal system. In the latter case a Wannier-functions approach is able to clearly disentangle the bands of interest from the rest of the manifold. Al(111) and Pd(111) surfaces are taken as examples of low and high work-function metals, contacted with a semiconducting (8,0) CNT. In all cases we find that a surface dipole forms that locally shifts the band structure of the CNT; control of this electrostatic dipole directly controls the SBH.

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Date submitted: 20 Nov 2009 Electronic form version 1.4