Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Adapting DFT C6-corrections for modeling graphene on metal surfaces[1] PETER SCHULTZ, Sandia National Laboratories, Albuquerque, NM, USA, MICHAEL FOSTER, Sandia National Laboratories, Livermore, CA, USA — Modeling graphene on metals accurately presents a challenge for first principles due to difficulties modeling non-local electron correlation. An effective model must resolve small van der Waals (vdW) binding of graphene to the surface from the large cohesive energy in the metal and chemical bond energies in the graphene. Conventional density functional theory (DFT) such as GGA/PBE fails to describe vdW effects accurately. More sophisticated non-local vdW functionals, still in their infancy, produce inconsistent results, and there is a shortage of experimental data to assess which of these is more reliable. Moreover, computational expense limits their general application. We adapt DFT plus C6-corrected methods in concert with non-local vdW functionals to study graphene on Cu(111), Ni(111), and Ir(111). The known strengths of vdW-functionals and limited experimental data are used to constrain the definition of the C6-corrections (which in turn provides guidance as to which vdW-enhanced functionals are most suitable for accurate simulations of graphene adsorption on metals). The less expensive DFT+C6 and vdW-DFT are shown to give consistent results, and agree with known experimental data for these three metal surfaces.

[1]Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Company, for the U.S. Department of Energy's NNSA under contract DE-AC04-94AL85000.

Peter Schultz
Sandia National Laboratories

Date submitted: 14 Nov 2014 Electronic form version 1.4