Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Comparative first-principles study of clean-surface properties of metals ABHIRUP PATRA, JIANWEI SUN, JOHN P. PERDEW, Department of Physics, Temple University — Metal surfaces are widely used in different applications from nano-devices to heterogeneous catalysis. Clean-surface properties such as the surface energy, work function and interlayer spacing importantly determine the behavior of metal surfaces. Prior work has been done to understand these properties using high-level methods including the local density approximation (LDA) and the generalized gradient approximation (PBE). In this work, we study (111) (100) and (110) surfaces of Pt, Pd, Cu, Al, Au, Ag, Rh and Ru by extrapolation from a finite number of layers. These surfaces are studied using SCAN, a new member of the computationally-efficient meta-GGA family of density functionals. We have compared the performance of SCAN and three other standard density functionals - LDA, PBE and PBEsol - to available experimental results. We find that the performance of the general-purpose SCAN is at the level of the more-specialized PBEsol, giving accurate metallic properties. Ref: Jianwei Sun, Adrienn Ruzsinszky, John P Perdew, Strongly Constrained and Appropriately Normed Semilocal Density Functional, *Physical Review Letters*115 (3), 036402 (2015). Supported by NSF under DMR-1305135, CNS-09-5884, and by DOE under DE-SC0012575, DE-AC02-05CH11231.

Abhirup Patra
Department of Physics, Temple University

Date submitted: 07 Nov 2015 Electronic form version 1.4