Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Accurate Energies and Orbital Description in Semi-Local Kohn-Sham DFT ALEXANDER LINDMAA, Linkoping University, STEPHAN KUEMMEL, University of Bayreuth, RICKARD ARMIENTO, Linkoping University —
We present our progress on a scheme in semi-local Kohn-Sham density-functional theory (KS-DFT) for improving the orbital description while still retaining the level of accuracy of the usual semi-local exchange-correlation (xc) functionals. DFT is a widely used tool for first-principles calculations of properties of materials. A given task normally requires a balance of accuracy and computational cost, which is well achieved with semi-local DFT. However, commonly used semi-local xc functionals have important shortcomings which often can be attributed to features of the corresponding xc potential. One shortcoming is an overly delocalized representation of localized orbitals. Recently a semi-local GGA-type xc functional was constructed to address these issues [1], however, it has the trade-off of lower accuracy of the total energy. We discuss the source of this error in terms of a surplus energy contribution in the functional that needs to be accounted for, and offer a remedy for this issue which formally stays within KS-DFT, and, which does not harshly increase the computational effort. The end result is a scheme that combines accurate total energies (e.g., relaxed geometries) with an improved orbital description (e.g., improved band structure). [1] PRL 111, 036402 (2013)

Alexander Lindmaa
Linkoping Univ - Linkoping

Date submitted: 13 Nov 2014 Electronic form version 1.4