Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

SCAN+rVV10: A promising van der Waals density functional[1]
HAOWEI PENG, ZENG-HUI YANG, JIANWEI SUN, JOHN PERDEW, Department of Physics, Temple Univeristy — The newly developed "strongly constrained and appropriately normed" (SCAN) meta-generalized-gradient approximation (meta-GGA) can generally improve over the non-empirical Perdew-Burke-Ernzerhof (PBE) GGA not only for strong chemical bonding, but also for the intermediate-range van der Waals (vdW) interaction. However, the long-range vdW interaction is still missing. To remedy this, we propose here pairing SCAN with the non-local correlation part from the rVV10 vdW density functional, with only two empirical parameters. The resulting *SCAN+rVV10* yields excellent geometric and energetic results not only for molecular systems, but also for solids and layered-structure materials, as well as the adsorption of benzene on coinage metal surfaces. Especially, SCAN+rVV10 outperforms all current methods with comparable computational efficiencies, accurately reproducing the three most fundamental parameters—the inter-layer binding energies, inter-, and intra-layer lattice constants—for 28 layered-structure materials. Hence, we have achieved with SCAN+rVV10 a promising vdW density functional for general geometries, with minimal empiricism.

[1]This work was supported as part of the Center for the Computational Design of Functional Layered Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under Award .DE-SC0012575.

Haowei Peng
Department of Physics, Temple Univeristy

Date submitted: 06 Nov 2015 Electronic form version 1.4