

TSF16-2016-000126

T

Abstract for an Invited Paper
for the TSF16 Meeting of
the American Physical Society

SCAN: An Efficient Density Functional Yielding Accurate Structures and Energies of Diversely-Bonded Materials

JIANWEI SUN, The University of Texas at El Paso

The accuracy and computational efficiency of the widely used Kohn-Sham density functional theory (DFT) are limited by the approximation to its exchange-correlation energy E_{xc} . The earliest local density approximation (LDA) overestimates the strengths of all bonds near equilibrium (even the vdW bonds). By adding the electron density gradient to model E_{xc} , generalized gradient approximations (GGAs) generally soften the bonds to give robust and overall more accurate descriptions, except for the vdW interaction which is largely lost. Further improvement for covalent, ionic, and hydrogen bonds can be obtained by the computationally more expensive hybrid GGAs, which mix GGAs with the nonlocal exact exchange. Meta-GGAs are still semilocal in computation and thus efficient. Compared to GGAs, they add the kinetic energy density that enables them to recognize and accordingly treat different bonds, which no LDA or GGA can [1]. We show here that the recently developed non-empirical strongly constrained and appropriately normed (SCAN) meta-GGA [2] improves significantly over LDA and the standard Perdew-Burke-Ernzerhof GGA for geometries and energies of diversely-bonded materials (including covalent, metallic, ionic, hydrogen, and vdW bonds) at comparable efficiency [3]. Often SCAN matches or improves upon the accuracy of a hybrid functional, at almost-GGA cost. [1] J. Sun et al., Phys. Rev. Lett. 111, 106401 (2013). [2] J. Sun et al, Phys. Rev. Lett. 115, 036402 (2015). [3] J. Sun et al., Nat. Chem. 8, 831 (2016).