Strongly Constrained and Appropriately Normed (SCAN) Semilocal Density Functional: Accurate and Efficient for Structures and Energies of Diversely-Bonded Materials

Jianwei Sun

Department of Physics

The University of Texas at El Paso

In condensed matter physics, materials science, and chemistry, it is of critical importance to know if one atom or molecule can bind to another and with how much energy. The strengths of different types of bonds between atoms and molecules can vary from several meV to several eV. Although some first-principles methods can provide accurate descriptions of all bond types, those methods are not efficient enough for studies of complex systems (e.g., large systems, *ab initio* molecular dynamics, and high-throughput searches for functional materials). We show here that the recently developed non-empirical strongly constrained and appropriately normed (SCAN) [1] meta-generalized gradient approximation (meta-GGA) within the density functional theory framework predicts accurate geometries and energies of diversely-bonded molecules and materials (including covalent, metallic, ionic, hydrogen, and van der Waals bonds), significantly improving over its predecessors, at comparable efficiency, the GGAs that dominate materials computation [2]. SCAN is the first meta-GGA that is fully constrained, obeying all 17 known exact constraints that a meta-GGA can. The meta-GGA is also exact or nearly exact for a set of "appropriate norms", where the exact exchange- correlation hole is localized near its electron. Remarkably, SCAN often matches or improves upon the accuracy of a computationally expensive hybrid functional, at almost-GGA cost. Two error sources, i.e., the long-range vdW interaction and the self-interaction error, intrinsic to any semilocal density functionals to which SCAN belongs, however remain. The addition of the long-range vdW correction to SCAN [3] results in a versatile vdW functional that is accurate and outperforms its competitors for a variety of vdW-dominated systems, including layered materials and organic molecules adsorbed on metal surfaces.

[1] J. Sun, A. Ruzsinszky, and J.P. Perdew, Strongly constrained and appropriately normed semilocal density functional, *PRL* **115**, 036402 (2015).

[2] J. Sun, R.C. Remsing, Y. Zhang, Z. Sun, A. Ruzsinszky, H. Peng, Z. Yang, A. Paul, U. Waghmare, X. Wu, M.L. Klein, and J.P. Perdew, Accurate First-principles structures and energies of diversely-bonded systems from an efficient density functional, *Nat. Chem.* **8**, 831 (2016).

[3] H. Peng, Z. Yang, J.P. Perdew, and J. Sun, Versatile van der Waals density functional based on a meta-generalized gradient approximation, *PRX* **6**, 041005 (2016).