LACNS

Louisiana Consortium for Neutron Scattering

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1008B Digital Media Center
Louisiana State University

The SCAN density functional and its surprising performance in cuprates

The accuracy and computational efficiency of the widely used Kohn-Sham density functional theory (DFT) is limited by the approximation to its exchange-correlation energy Exc. 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 Exc, 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 [2]. In this talk, I will present an advance in DFT, the recently developed non-empirical strongly constrained and appropriately normed (SCAN) meta-generalized gradient approximation (meta-GGA) [1]. SCAN 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, the GGAs that dominate materials computation, at comparable efficiency [2]. SCAN's excellent performance on cuprates, traditionally regarded as strongly-correlated systems out of reach of DFT, will be highlighted, exemplified by its accurate prediction of the metal insulator transition of La_2CuO_4 under doping [3]. I will further explain how SCAN was constructed [1], why it can improve over GGAs [2], and where it should fail [4]. At the end, efforts to improve SCAN via nonlocal corrections will be discussed.

[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] J.W. Furness, Y. Zhang, C. Lane, I.G. Buda, B. Barbiellini, R.S. Markiewicz, A. Bansil, and J. Sun, An accurate first-principles treatment of doping-dependent electronic structure of high-temperature cuprate superconductors, *Nature Communication Physics*, **1**, 11 (2018).

[4] 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).

Guest Speaker

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