Tests of Local Functionals for Predicting Condensed-Phase Structural and Electronic Properties, Including Nanoporous Materials

Indrani Choudhuri
University of Minnesota

The accurate determination of structural parameters (lattice constants, unit cell volumes, pore sizes, bond lengths, bond angles, and torsional angles) is necessary for understanding the electronic and magnetic properties of MOFs and other semiconducting and insulating solids. For this purpose, it is especially interesting to test local functionals because their cost is more affordable in plane wave calculations and in Gaussian calculations for large systems.

For structural aspects of nanoporous solids, a diverse group of local exchange-correlation functionals (MN15-L, revM06-L, PBE, PBEsol, PBE-D2, PBE-D3, VdW-DF2, revTPSS, SCAN, and SOGGA) is applied to a very diverse test set of 12 metal organic frameworks (MOFs). The recent functionals revM06-L [Wang, Jin, Yu, Truhlar, and He, PNAS 2017], which is a reparametrized version of M06-L, and SCAN [Sun, Ruzsinszky, and Perdew, PRL 2015] are found to be the two most accurate functionals for predicting structural parameters.

For the study of band gaps, another recently developed local exchange-correlation functional, HLE17 [Verma and Truhlar, JPC C 2019], is tested for various kinds of semiconductors, including metal organic frameworks (MOFs), covalent organic frameworks (COFs), perovskites, zeolites, and others. The HLE17 functional is distinguished by having high local exchange. It is found to be more accurate then PBE, PBEsol, and PBE+U and almost as accurate as the much more expensive HSE06. For the MOFs, HLE17 is as accurate as HSE06 with almost 100 times less computational cost.