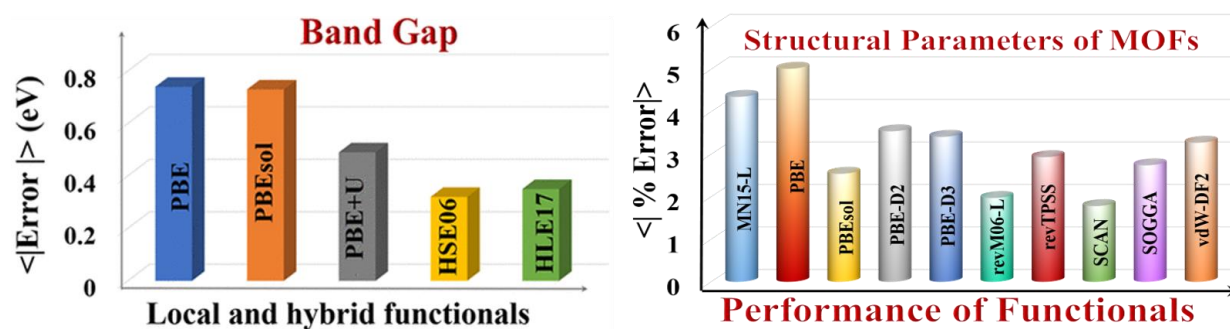


Tests of local functionals for predicting condensed-phase structural and electronic properties, including nanoporous materials

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 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 MOFs. The recent functionals revM06-L (reparametrized version of M06-L) and SCAN are found to be the two most accurate functionals for predicting structural parameters.¹

For the study of band gaps, another recently developed local exchange-correlation functional, HLE17, is tested for various kinds of semiconductors, including metal organic frameworks (MOFs), covalent organic frameworks (COFs), perovskites, zeolites, and others. HLE17 is found to be more accurate than 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.²



1. Choudhuri, Truhlar. to be published.

2. Choudhuri, Truhlar. *J. Phys. Chem. C* **2019**, *123*, 28, 17416-17424