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Benchmarking of the Density Functional Theory Methods for Accurate Description of Structural Properties in Metal-Organic Frameworks

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Atomic level simulations, such as molecular dynamics (MD), Monte Carlo (MC) or DFT, have recently become indispensable tools for characterization of porous materials [1]. Computational methods are often used to study adsorption, diffusion or separation mechanisms. Here, we perform density functional theory (DFT) calculations of structural properties of flexible and rigid nanoporous MOFs. For the benchmarking for comparison we chose materials from the family of MIL-53 with different metallic centers (Al, Fe, Sc) and flexible materials from the group of zeolitic imidazolate frameworks (ZIF) - ZIF-4, ZIF-8. Additionally, rigid frameworks (IRMOF-1, HKUST-1, Mg-formate and Zn-MOF-74) were added. To describe the interactions in our systems we have selected well-known generalized gradient approximation of exchange-correlation functionals based on PBE functional developed by Pedrew et. al. [2]. Empirical dispersion corrections (D2 and TS) impact on the selected model was also analyzed [3].
We compared the calculated lattice parameters, bond lengths and angels with well-defined experimental structures obtained from low-temperature X-ray powder diffraction (Fig. 1.). The results of our analysis can help to select the best-describing model for theoretical studies of MOFs and can also be a starting point for other applications of DFT methods such as construction of a force field for MD or MC calculations.

References

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