Development of Efficient Ab Initio method to Characterize Porous materials

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Porous materials are promising for a wide selection of energy and environmental related applications. Since the number of distinct porous materials that can be experimentally synthesized is exceedingly large, computational characterization of porous materials prior to experimental synthesis can play an important role in materials development. In this work, we have developed a new efficient method based on ab initio calculation, to accurately and efficiently characterize adsorption properties of porous materials. We applied our method for CO_2, CH_4 and N_2 adsorption in Mg and Zn-MOF-74, which have open metal site. We demonstrate that our method recover most of the interesting adsorption properties without developing classical force fields. Furthermore, we discover that the binding energy value is not sufficient when evaluating material performance in certain cases. We expect that our method can be applied to many other systems and be used to screening a large number of porous materials.