Evaluation of Metal-Organic Framework Forcefields for Methane Storage and Delivery

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Metal-organic frameworks (MOFs) are a class of nanoporous materials assembled from metal clusters and organic ligands. Due to their large internal surface area and tunability, many studies were performed to find well-performing structures for various applications. Recently, with tens of thousands of structures synthesized, it is important to find application fields of MOFs already known. Molecular simulations have become an important tool to quickly determine high-performing MOFs. Prediction of adsorption performance of a given material depends critically on the molecular model, however, current high-throughput computational screening relies on using the off-the-shelf forcefields that has not been optimized for this purpose. In this work, we evaluated the reliability of the off-the-shelf forcefields, such as UFF, on predicting the ranking from a list of materials. Our results show that the off-the-shelf forcefields do not accurately predict the relative ranking of these materials. To improve the prediction, we developed a new forcefield for methane adsorption that can improve the prediction of relative ranking of these materials using machine learning methods, and metaheuristics.