TITLE: High Throughput Computational Prediction of Gas Separation Properties of Metal Organic Frameworks (MOFs)

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ABSTRACT BODY:

There is a widespread interest in application of metal organic frameworks for gas separation processes. A tremendous amount of research has been devoted in designing and synthesizing MOFs that are optimum for gas separation processes. In past few years, the number of synthesized MOFs has increased exponentially, which makes it impossible to experimentally test each MOF for a particular application. Hence, there is a need for a tool which can quickly evaluate the structure property relationships of various MOFs and identify promising candidates.

In this work, high-throughput computational methods have been used to evaluate adsorption, selectivity and permeability of CO_2 and N_2 for an existing database of hypothetical MOFs (Wilmer et al.)[1] containing over 137,000 MOFs. Thus obtained results are analyzed for structure-functional relationships such as dependencies on MOF chemistry, void fraction, pore limiting diameter (PLD) and the largest cavity diameter (LCD). In the future, thus obtained properties will be used to determine gas separation properties of mixed matrix membranes containing MOFs as filler particles.

[1] C. E. Wilmer, M. Leaf, C. Y. Lee, O. K. Farha, J. T. Hupp, B.G. Hauser, R.Q. Snurr, Nature. Chem. 4(2012), 83.