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PyCOSMOS: A Python Tool for Compartmentalization of Unit Cells of Metal-Organic Frameworks

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Metal-Organic Frameworks (MOFs) stand out as a prominent class of nanoporous materials, known for their stability and customizable pore sizes and chemistry, particularly for gas storage and separations. Notably, certain MOFs exhibit pH sensitivity, rendering them excellent candidates for drug delivery applications. The precise characterization of MOFs is of paramount importance for effective design and synthesis for a given application.

Real MOF samples often deviate from ideal crystals due to presence of binders, residual solvents, and pore blockage defects. To characterize this non-ideality at the pore level, we recently introduced the method of calculating pore accessibilities by comparing the in silico calculated fingerprint isotherms and experimental isotherms.1 However, accurate calculation of fingerprint requires knowledge of the shape, size and location of the pore which can be difficult to deduce from the structure alone. In this work, we developed a python program, pyCOSMOS, to describe the shape, size, and location of the pores of MOFs.2 Using the pore size distribution probe particles as input, a special clustering algorithm identifies the pores of different types. Later, the unit cell is decomposed into pore compartments, and Monte Carlo simulations of gas adsorption are performed for calculating the fingerprint isotherms. The generalizability of the program is demonstrated by application to most practical MOFs like Cu-BTC, IRMOF-1, UiO-66, PCN-224, ZIF-412, as well as various structures from the CoRE MOF database.

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1. Parashar, S.; Zhu, Q.; Dantas, S.; Neimark, A. V., Monte Carlo Simulations of Nanopore Compartmentalization Yield Fingerprint Adsorption Isotherms as a Rationale for Advanced Structure Characterization of Metal–Organic Frameworks. ACS Applied Nano Materials 2021, 4 (5), 5531-5540.

2. Parashar, S; Neimark, A.V.; Pore Structure Compartmentalization for Advanced Characterization of Metal-Organic Framework Materials. Theo. & Comp. Chem. ChemRxiv. 2023.

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