Identification of MOFs with Unique Pore Shapes Using Computer Vision

Saad Aldin Mohamed and Jianwen Jiang*

Department of Chemical and Biomolecular Engineering, National University of Singapore, 117576, Singapore

**Correspondence to:* chejj@nus.edu.sg

Computer vision holds great promise for accelerating the discovery of porous materials, including metal–organic frameworks (MOFs). It can support MOF synthesis and enable identification of resulting crystal morphologies. At the atomistic level, generating MOF images combined with modern computer vision approaches such as, convolutional neural networks (CNN), enables mapping of porosity and framework topology to material's adsorption properties. Here, we apply computer vision to distinguish pore shapes in MOFs for shape-matching separation. In particular, separation of xylene isomers is a very challenging process due to their similar physicochemical properties. We present a computer vision–driven workflow to rapidly identify MOFs with one-dimensional (1D) triangular pores that can preferentially accommodate the shape matching *m*–xylene (*m*X) over *p*–xylene (*p*X) and *o*–xylene (*o*X). The proposed workflow is illustrated in Figure 1. Starting from pristine CIFs in a large experimental MOF database, we generated 2D voxelized images by projecting each crystal along its 1D pore direction. A contour detection was then used to isolate the shape from the generated MOF images and classified them using polygon approximation. In parallel, CNN autoencoder was used to learn a latent representation for MOF images, followed by clustering MOF images with similar pore shapes. Finally, the identified MOFs with triangular pores were subjected to multicomponent adsorption simulations, shortlisting novel candidates wherein *m*X wedges at the vertex of their triangular pores leading to notable *m*X selectivity. This study demonstrates that computer vision can help in the discovery of porous materials with unique pore shapes for practical applications.

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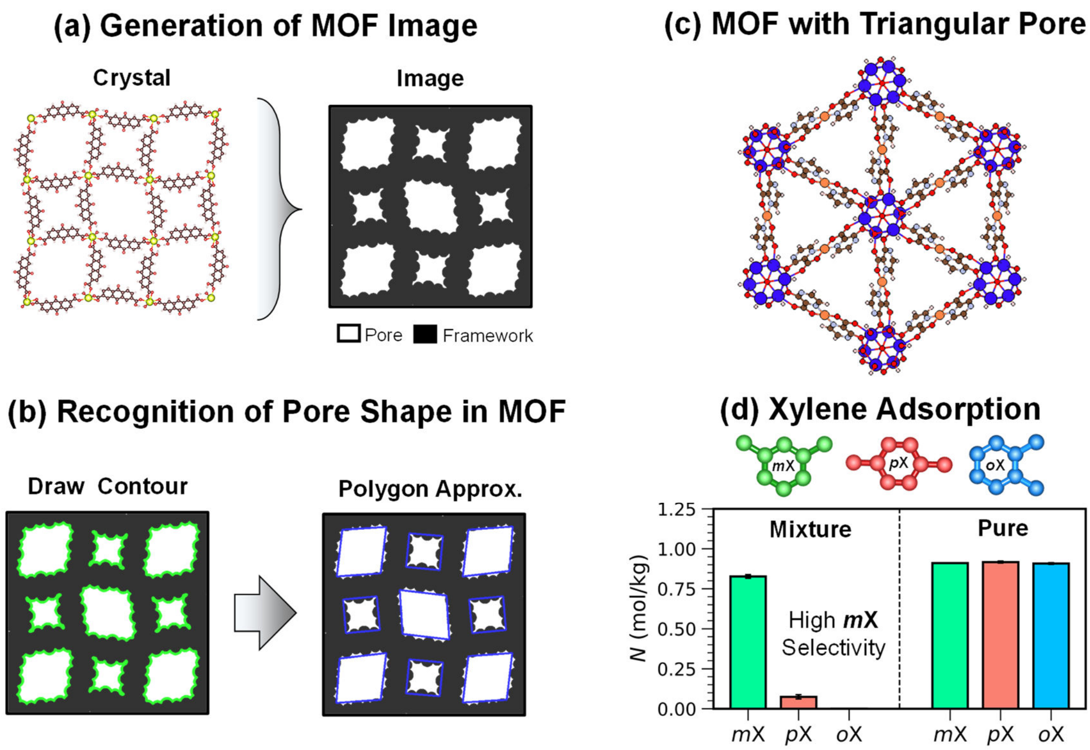

Figure 1: Workflow to identify MOFs with unique pore shapes. **(a)** Generation of MOF images from crystal structures. **(b)** Detection and classification of pore shape in MOF images. **(c)** Identification of MOFs with triangular pores. **(d)** Selective *m*–xylene (*m*X) adsorption in MOFs with triangular pores.