

Pore Size Distribution Prediction of MOFs Using Machine Learning Approach

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Pore size distribution (PSD) is one of the most critical properties to characterize nanoporous materials, especially for chemical separation. The current state-of-the-art techniques for obtaining the PSD use an adsorption isotherm as an input to various methods, such as Horvath-Kawazoe (HK), Barrett-Joyner-Halenda (BJH), non-local density functional theory (NLDFT), and quench solid density functional theory (QSDFT), developed for idealized surfaces. The adsorption community has widely adopted and routinely used these methods in the literature to characterize new and already synthesized nanoporous materials. However, recent studies in the literature show that these well-established methods can be sensitive to small structural defects. Toward this end, in this work, we developed a machine learning (ML) approach to predict the PSD of a class of nanoporous materials such as metal-organic frameworks. We compared and discussed the developed ML model with the current state-of-the-art methods.