Improve Pore Size Distribution Calculation in Nanoporous Materials With Machine Learning Approach

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Pore size distribution (PSD) is one of the most critical properties to characterize nanoporous materials, especially for gas storage and 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, BJH, and Non-Local Density Functional Theory. The adsorption community has widely adopted and routinely used these methods in the literature to characterize new and already synthesized nanoporous materials. However, recent study in the literature show that these well-established methods can be sensitive to small structural defects. Toward this end, in this work, we developed machine learning (ML) approach to predict the PSD properties of a class of nanoporous materials such as metal-organic frameworks (MOFs). We compared and discussed the developed ML models with the current state-of-the-art methods.