

Big Data and Machine Learning for Nanoporous Materials Characterization and Discovery



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ABSTRACT: Big data and machine learning methods are revolutionizing the field of chemistry, material science, and chemical engineering. In this talk, I will discuss how the development of the nanoporous materials database could help develop a machine learning approach to resolve some of the issues that the Brunauer-Emmett-Teller (BET) method -- the most widely used surface area characterization technique in the world -- had in characterizing the nanoporous materials with both micro and mesopores. Additionally, I will show how the dataset could be combined with virtual high-throughput screening to discover high-performing nanoporous materials for C₂ gas separation, which was subsequently synthesized and tested.