Data-driven discovery and multi-scale modeling of nanoporous materials for energy and environmental applications

Abstract

Nanoporous materials, such as zeolites, metal-organic frameworks (MOFs), and porous organic polymers (POPs), offer transformative potential for various energy and environmental applications, such as gas storage, separation, and carbon capture. However, the vast chemical and material space for synthesis represents both opportunities and challenges in identifying optimal materials for specific applications.

In this talk, I will discuss how molecular simulations combined with artificial intelligence (AI) and data science have accelerated design, characterization, and screening of nanoporous materials. We will explore the evolution of experimental MOF database (CoRE MOF database) and how they have accelerated high-throughput screening for separation applications. Additionally, I will highlight the integration of data-driven approaches, such as AI, complement traditional computational methods to expedite the design and characterization of amorphous nanoporous materials, such as porous organic polymers.

Finally, I will discuss the importance of multi-scale modeling and simulation in assessing material's performance under realistic scenarios, including complex multi-component gas separations, boil-off gas capture, and carbon capture applications.

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