

## **Advances in high-throughput screening and design of MOFs using machine learning**

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Metal-organic frameworks (MOFs) are attractive materials for applications in gas storage and separations owing to their high porosity and surface area. However, due to the vast combinations of nodes, linkers, and topologies that can form unique MOFs, there are a virtually unlimited number of possible MOFs that can be envisioned. In this talk, I will explore how computational screening has accelerated the discovery of useful MOFs for gas storage and separations and how machine learning tools can be used to accelerate this screening even further. I will also introduce advances in using a variational autoencoder to design novel MOFs with applications in carbon capture.