High-throughput computation and data science for metal-organic framework (MOF) and covalent-organic framework (COF) materials

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Metal–organic frameworks (MOFs) and covalent-organic frameworks (COFs) offer unprecedented structural and chemical tunability, making them excellent platforms for gas sensing and separation. However, optimizing their properties requires navigating vast chemical search spaces and understanding complex multiscale phenomena. This presentation highlights how integrating high-throughput simulations and data science techniques can enhance our mechanistic understanding of MOF-based technologies.

First, we address the challenge of non-invasive disease diagnosis via human breath analysis. Using a newly developed high-throughput computational protocol, we evaluate the sensing efficacy of MOF–metal oxide chemiresistive composites toward over 100 volatile organic compound biomarkers spanning 13 diseases. By combining cluster-based structure relaxation, binding energy informatics, and electronic density-of-states comparisons via Wasserstein distances, we obtain insights into the sensing mechanism and identify new directions for preventative medicine (Nurhuda *et al. Adv. Theory Simul.* 2025, **8**, 2401404).

Second, we explore computational workflows for predicting gas adsorption metrics across large structural databases. Focusing on COFs, we demonstrate how machine learning models trained on structural features, functionalization patterns, and interlayer shifts can rapidly predict Henry coefficients and adsorption thermodynamics for both polar and nonpolar gases. Importantly, our models and structural features are specifically selected to be physically interpretable, providing deeper insights into the gas uptake mechanism (Nurhuda *et al. Adv. Theory Simul.* 2026, **9**, e00003).

Finally, we consider composite materials by examining gas separation and gas transport in MOF-polymer mixed-matrix membranes (MMMs). Using atomistic simulations of steady-state CO_2/N_2 fluxes through MUF-16-based MMMs, as well as novel time-domain analysis, we reveal non-averaging dynamic phenomena emerging at the polymer–MOF interface. We show that the slow collective modes of the MOF are reshaped upon composite formation, gas-flux coupling rises beyond pure-phase averages, and kinetic behaviors shift in a gas-specific manner. These insights highlight the critical role of interfacial dynamics in membrane design, and confirm that static structure is insufficient for understanding gas transport in composite materials (Meza *et al. Manuscript in preparation*).