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Computational Discovery of Metal-Organic Frameworks for CO_2 Capture and Energy Storage DONALD SIEGEL, Univ of Michigan - Ann Arbor — Because of their high surface areas, crystallinity, and tunable properties, metal−organic frameworks (MOFs) have attracted intense interest as materials for gas capture and energy storage. An often-cited benefit of MOFs is their large number of possible structures and compositions. Nevertheless, this design flexibility also has drawbacks, as pinpointing optimal compounds from thousands of candidates can be time consuming and costly using experimental approaches. Consequently, computational approaches are garnering increasing importance as a means to accelerate the discovery of high-performing MOFs. Here we combine several computational techniques to identify promising MOFs for CO_2 capture and the storage of gaseous fuels (methane and hydrogen). The techniques include: (*i*) high-throughput screening based on data-mining and empirical correlations [1]; (*ii*) Monte Carlo simulations based on quantum-mechanically-informed forcefields [2,3]; and (*iii*) first-principles calculations of thermodynamics and electronic structure [4,5]. For CO_2 capture and CH_4 storage, these techniques are used to explore metal-substituted variants of M-DOBDC and M-HKUST-1. In the case of H_2, we identify trends and promising adsorbents amongst 4,000 compounds mined from the Cambridge Structure Database.

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