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Developing Effective Sorbents for Direct Air Capture using Large-scale DFT Calculations and ML Forcefields

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Previous high-throughput computational modeling of crystalline sorbents relevant for Direct Air Capture (DAC) has typically relied on empirical forcefields (FFs), approximated sorbent structures as being rigid, and often considered only adsorption of CO2. These assumptions are unlikely to be appropriate in developing practical DAC sorbents, which involve coadsorption of CO2 and H2O in configurations that include chemical complexation and structural rearrangement of adsorbent microenvironments. To address these limitations, we have generated a data set with tens of millions of DFT calculations examining adsorption of CO2 and/or H2O in a diverse collection of metal-organic frameworks, including many materials with chemically-relevant point defects. This talk will discuss uses of this data set for directly identifying useful sorbents for DAC and also for developing machine learning FFs that can describe the full spectrum of adsorption in MOFs.

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References

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