in silico discovery of nanoporous materials for CO_2 capture and CoRE MOF database

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Discovery of new adsorbent materials with large CO_2 working capacity could help reduce CO_2 emissions from newly commissioned power plants using pre-combustion carbon capture. High-throughput computational screening efforts can accelerate the discovery of new adsorbents but sometimes require significant computational resources to explore the large space of possible materials. Here, we report in silico discovery of high-performing adsorbents for pre-combustion CO_2 capture by applying a genetic algorithm (GA) to efficiently search a large database of metal-organic frameworks (MOFs) for top candidates. One of the synthesized MOFs shows a higher CO_2 working capacity than any MOF reported in the literature at the operating conditions investigated here.

We also report an updated version of the MOF database, namely, CoRE MOF Version 2.0, which can help accelerate the discovery of novel adsorbent materials for various of gas separation and catalytic applications.