Abstract Submitted
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Computational Design of Metal–Organic Frameworks with High Methane Deliverable Capacity[1] YI BAO, Rice University, RICHARD MARTIN, Lawrence Berkeley National Laboratory, CORY SIMON, University of California, Berkeley, MACIEJ HARANCZYK, Lawrence Berkeley National Laboratory, BEREND SMIT, University of California, Berkeley, MICHAEL DEEM, Rice University, DEEM TEAM, HARANCZYK TEAM, SMIT TEAM — Metal–organic frameworks (MOFs) are a rapidly emerging class of nanoporous materials with largely tunable chemistry and diverse applications in gas storage, gas purification, catalysis, etc. Intensive efforts are being made to develop new MOFs with desirable properties both experimentally and computationally in the past decades. To guide experimental synthesis with limited throughput, we develop a computational methodology to explore MOFs with high methane deliverable capacity. This *de novo* design procedure applies known chemical reactions, considers synthesizability and geometric requirements of organic linkers, and evolves a population of MOFs with desirable property efficiently. We identify about 500 MOFs with higher deliverable capacity than MOF-5 in 10 networks. We also investigate the relationship between deliverable capacity and internal surface area of MOFs. This methodology can be extended to MOFs with multiple types of linkers and multiple SBUs.

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