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In Silico Discovery of High Deliverable Capacity Metal-Organic Frameworks[1] YI BAO, Rice Univ, RICHARD MARTIN, Lawrence Berkeley National Lab, CORY SIMON, UC Berkeley, MACIEJ HARANCZYK, Lawrence Berkeley National Lab, BEREND SMIT, UC Berkeley, MICHAEL DEEM, Rice Univ, MICHAEL W. DEEM TEAM, MACIEJ HARANCZYK TEAM, BEREND SMIT TEAM — Metal organic frameworks (MOFs) are actively being explored as potential adsorbed natural gas storage materials for small vehicles. Experimental exploration of potential materials is limited by the throughput of synthetic chemistry. We here describe a computational methodology to complement and guide these experimental efforts. The method uses known chemical transformations *in silico* to identify MOFs with high methane deliverable capacity. The procedure explicitly considers synthesizability with geometric requirements on organic linkers. We efficiently search the composition and conformation space of organic linkers for nine MOF networks, finding 48 materials with higher predicted deliverable capacity (at 65 bar storage, 5.8 bar depletion, and 298 K) than MOF-5 in four of the nine networks. The best material has a predicted deliverable capacity 8% higher than that of MOF-5.

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