Covalent organic frameworks for carbon capture

They screen a database of more than 69,000 hypothetical covalent organic frameworks (COFs) for carbon capture, using parasitic energy as a metric. In order to compute CO2-framework interactions in molecular simulations, we develop a genetic algorithm to tune the charge equilibration method and derive accurate framework partial charges. Nearly 400 COFs are identified with parasitic energy lower than that of an amine scrubbing process using monoethanolamine; over 70 are better performers than the best experimental COFs; and several perform similarly to Mg-MOF-74. We analyze the effect of pore topology on carbon capture performance in order to guide development of improved carbon capture materials.