Covalent organic frameworks for methane storage applications

We present **69,840 covalent organic frameworks** (COFs) assembled *in silico* from a set of 666 distinct organic linkers into 2D layers and 3D networks. We investigate the feasibility of using these COFs for methane storage by using grand-canonical Monte Carlo (GCMC) simulations to calculate their deliverable capacities (DCs).

This interactive figure allows to explore the full database of assembled COF structures, together with their properties. All structures and properties can be downloaded in bulk from the Materials Cloud archive entry linked above.