

## CURATED covalent organic frameworks database

"Clean, Uniform, Refined with Automatic Tracking from Experimental Database" (CURATED) of Covalent Organic Frameworks (COFs).

- 324 COFs parsed from the literature and conveniently labelled
- 308 provided with DFT-optimized unit cell and geometry, with DDEC partial charges for molecular simulations (14 excluded because they contain counter-ions, 2 failed the DFT calculation)
- geometric pore properties computed for both the original and the optimized structures
- 296 porous COFs evaluated for Carbon Capture & Storage (CCS), considering simulated CO<sub>2</sub> and N<sub>2</sub> isotherms.

**Note: Charged structures (i.e., containing counterions) are excluded from the DFT optimization and non-porous structures are further excluded from CCS evaluation.**