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"H_2 sponge: pressure as a means for reversible high-capacity hydrogen storage in nanoporous Ca-intercalated covalent organic frameworks FEI GAO, Beijing Computational Science Res Ctr — We explore the potential and advantages of Ca-intercalated covalent organic framework-1 (CaCOF-1) as a 3 dimensional (3D) layered material for reversible hydrogen storage. Density functional theory calculations show that by varying the interlayer distance of CaCOF-1, a series of metastable structures can be achieved with the interlayer distance falling in the range of 4.3–4.8 . When four hydrogen molecules are adsorbed on each Ca, a high hydrogen uptake of 4.54 wt% can be produced, with the binding energy falling in the ideal range of 0.2–0.6 eV per H_2. While H_2 absorption is a spontaneous process under H_2 rich conditions, tuning the interlayer distance by reasonable external pressure could compress CaCOF-1 to release all of the hydrogen molecules and restore the material to its original state for recyclable use. This provides a new method for gradual, controllable extraction of hydrogen molecules in covalent organic frameworks, satisfying the practical demand for reversible hydrogen storage at ambient temperatures.

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