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# Hydrogen bonded Frameworks for CO2 capture and more

Hydrogen bonded frameworks (HOFs) have been known for a long time. In recent times, there has been enormous interest in their rational design from a wide library of hydrogen bonding molecules with varying geometries. Among the porous materials, molecular crystals bring advantageous features in terms of synthesis, solution processability and facile regeneration via recrystallization. However, generally they are made up of flexible components and the organic molecules can have many packing possibilities giving rise to unpredictable crystal structures. Yet, rational design of of uni- or binary-component H-bonded frameworks are being achieved and in some cases their use in applications such as gas separation, chiral resolution and ion sensing have been demonstrated. In general, HOFs are linked via a range of non-covalent interactions such as hydrogen bonds, halogen-directed weak interactions and different types of π–π interactions.

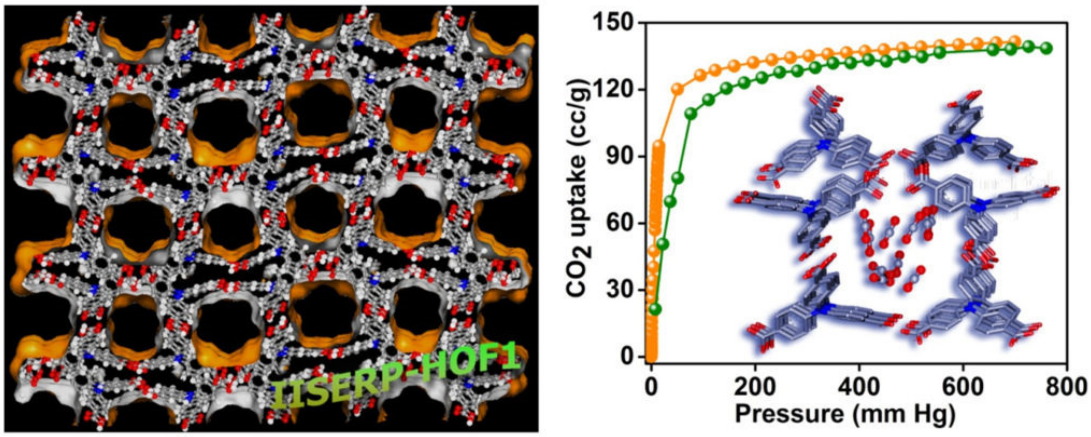


Fig. 1. Left: A Connolly surface representation of IISERP-HOF1. Right: Carbondioxide Adsorption isotherms of the HOF (Orange- Experimental; Green- Simulated.), with an inset showing CO2 within the nanopore of the HOF.

Here, we see HOFs also as excellent models for trapping gases and other small molecule guests and mining the information about the interaction of such species with these *metal-free organic frameworks* could bring some exceptionally valuable insights for designing not only HOFs but other advanced porous materials such as Metal Organic Framework (MOF), Covalent Organic Framework (COF) and Porous Organic Frameworks (POF), the amorphous analogues of COF. For example, in this work we have controlled the supramolecular hydrogen bonding assembly of a single tricarboxylate molecule via atomic manipulation. This approach is very effective as the complex set of vectors involved in the design is now simplified largely. It is like having to operate just one-level gear in your car for cruising. To this target, we have developed a 3-D hydrogen bonding network with one single molecule, which not only shows good $CO_2$ uptakes, but serves as a suitable model for realizing the different range of framework-$CO_2$ interactions. In future, we are planning to design more HOFs with this single or at most two-component assembly and investigate their interactions with a variety of guest species. Such methodology would provide a wealth of information for rational design of superior host frameworks in porous solids.

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## Publication

A permanently porous single molecule H-bonded organic framework for selective CO2 capture.
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