Examination of the Physical Aspects of Hydrogen Storage in MOFs

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Project ID #
STP39 Yaghi

Overview

Timeline

- Project start date
  1/1/2005
- Project end date
  12/31/2009
- Percent complete
  2.5%

Budget

- Total project funding
  - DOE share: $ *1.75M*
  - Contractor share: $ *0.437M*
- Funding received in FY04
  - $0.00
- Funding for FY05
  - $62,500

Barriers

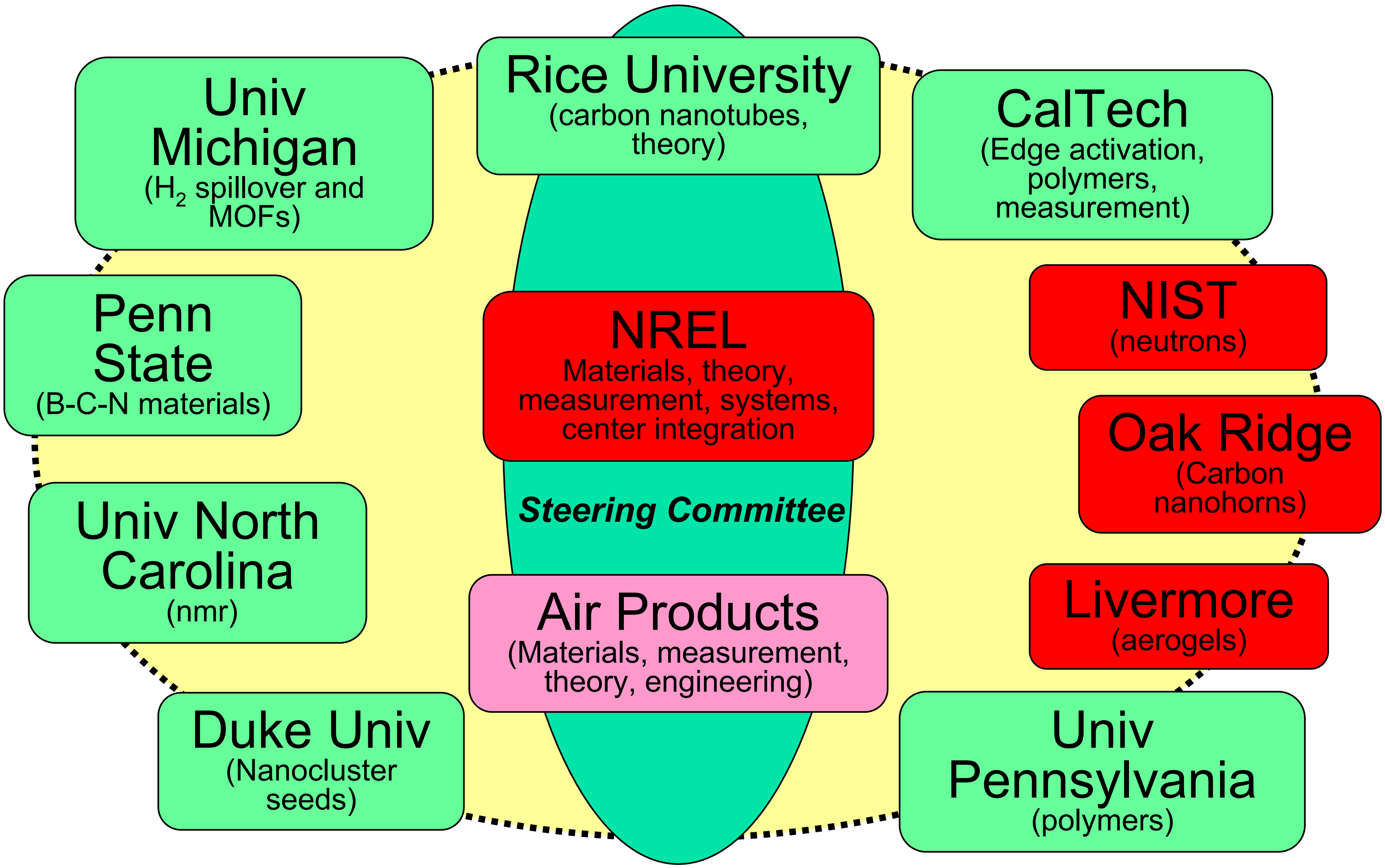
- Technical barriers addressed
  - **B) Weight and Volume**
  - **C) Efficiency**
  - **M) Hydrogen Capacity and Reversibility**
  - **N) Lack of Understanding of Hydrogen Physisorption and Chemisorption**
- Technical targets by YR 2010
  - **Gravimetric capacity: 6.0%**
  - **Volumetric capacity: 4.5%**
  - **Operating ambient temp.: -30/50 °C**
  - **Cycle life: 1000**

Partners

- NREL Team
- Yue Wu (University of North Carolina)
- Hansong Chen (Air Products)

CbHS Center of Excellence Partners

9 university projects (at 7 universities), 4 government labs, 1 industrial partner



Objectives

To develop novel, highly porous metal-organic framework materials (MOFs) as high capacity sorbents for H_2 storage applications.

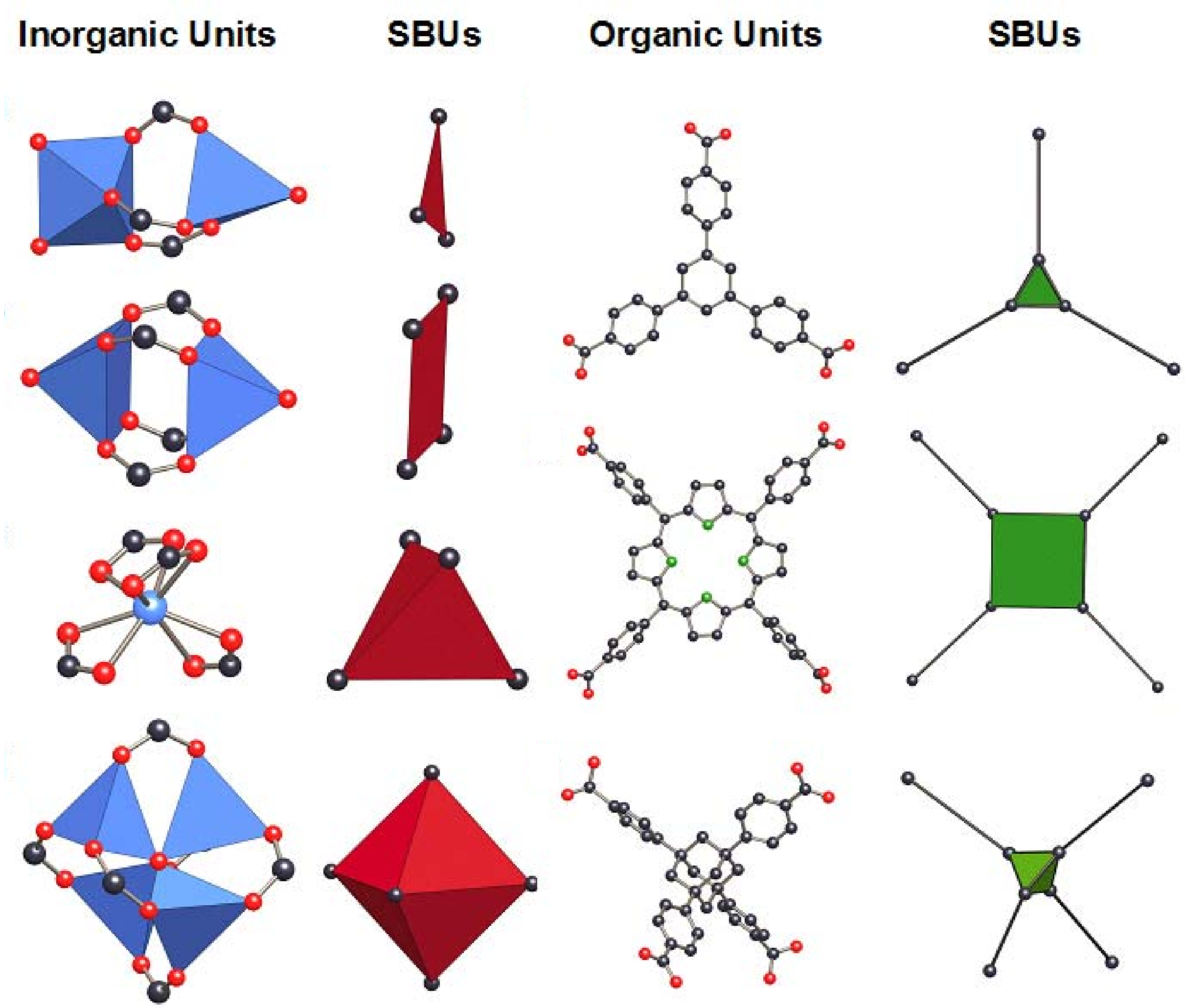
- Assess gravimetric and volumetric H_2 storage capacities of MOFs.
  - Explore pressure and temperature dependence of H_2 uptake in existing MOF materials over the parameter range specified in DOE YR2010 guidelines.
- Determine the optimal pore size and functionality for H_2 sorption and release in MOFs.
  - Characterize H_2 adsorption sites in existing MOF materials.
  - Study the relationship between pore size and level of H_2 uptake.

Approach

- Equilibrium H_2 uptake as a function of structure.
  - Survey hydrogen uptake levels in existing MOFs, under a variety conditions, to determine promising materials.
  - Use Raman Spectroscopy to probe in H_2 sorbed in pores.
- Correlate systematic changes in organic links with uptake.
  - Use above results to aid design of new structures with greater hydrogen storage capacities.
  - Synthesize new organic linkers and the corresponding MOFs.
  - Measure equilibrium H_2 uptake.

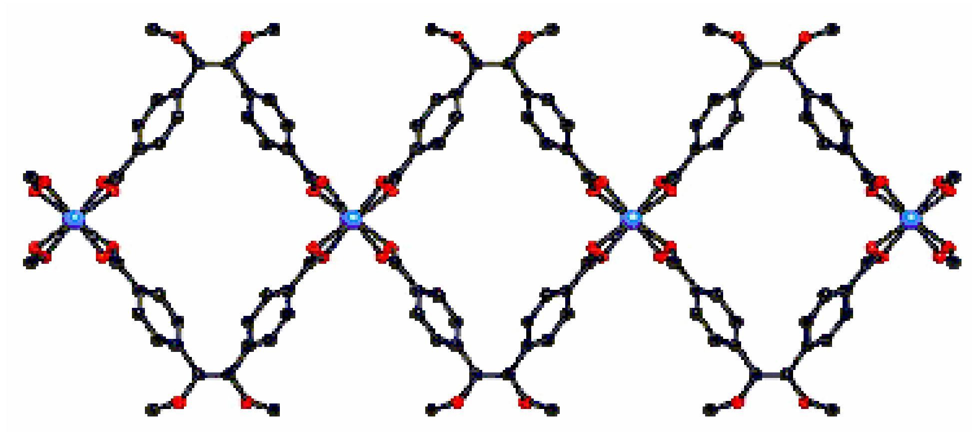
General Synthetic Strategy of MOFs

Cluster building block + Organic Link ⟶ MOF

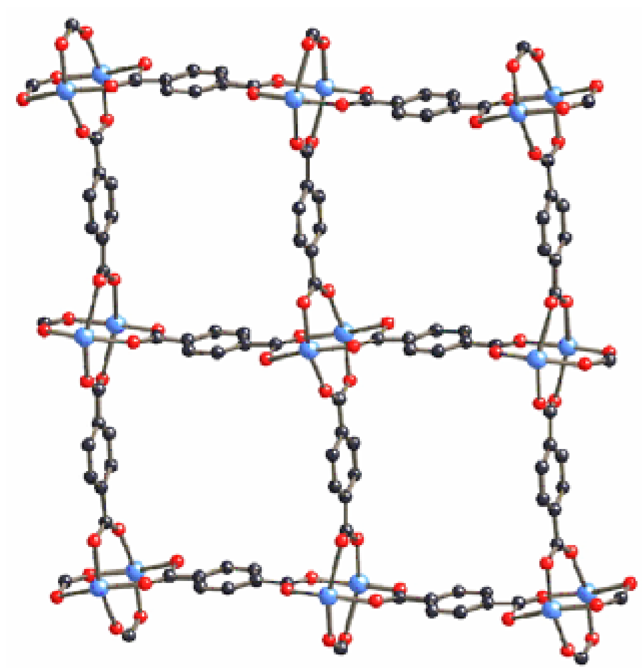


Control of MOF Dimensionality

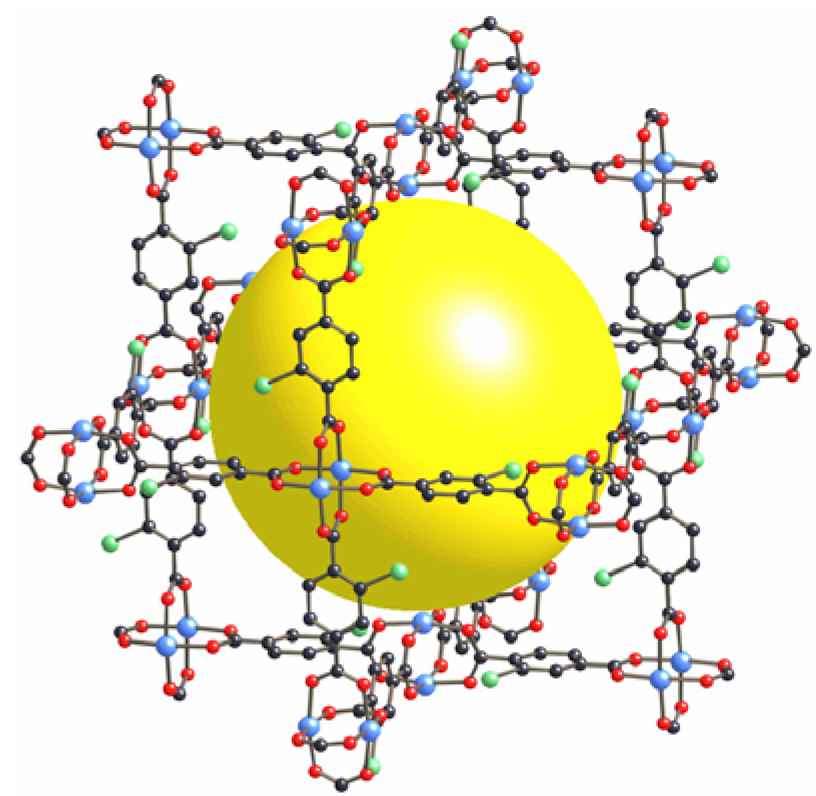
1D



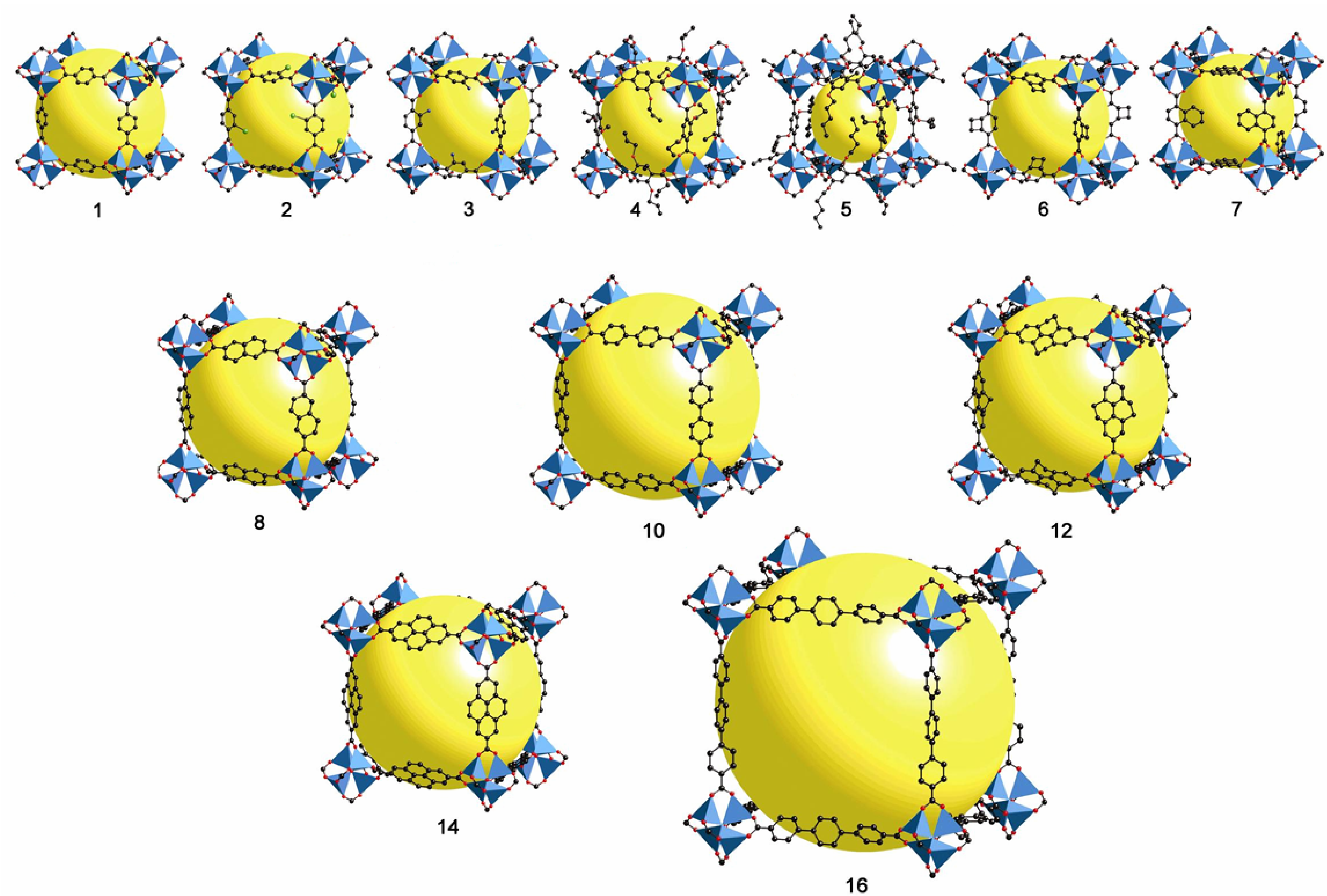
2D



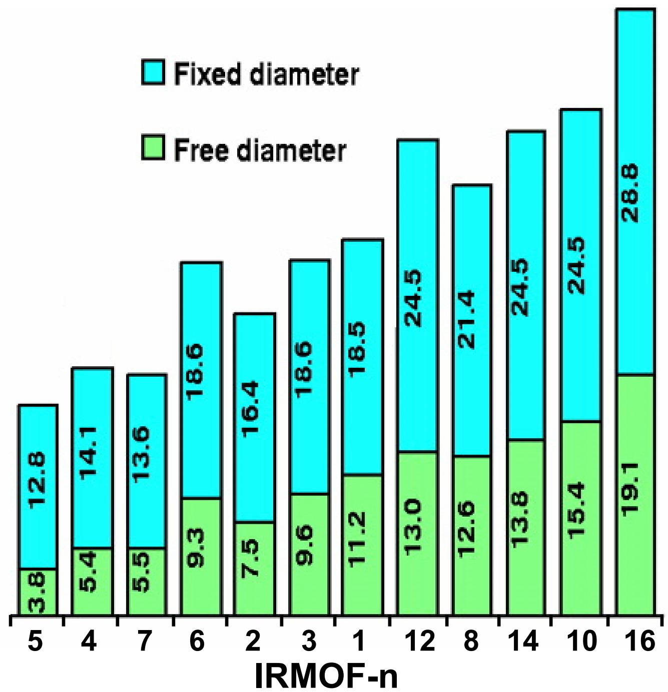
3D

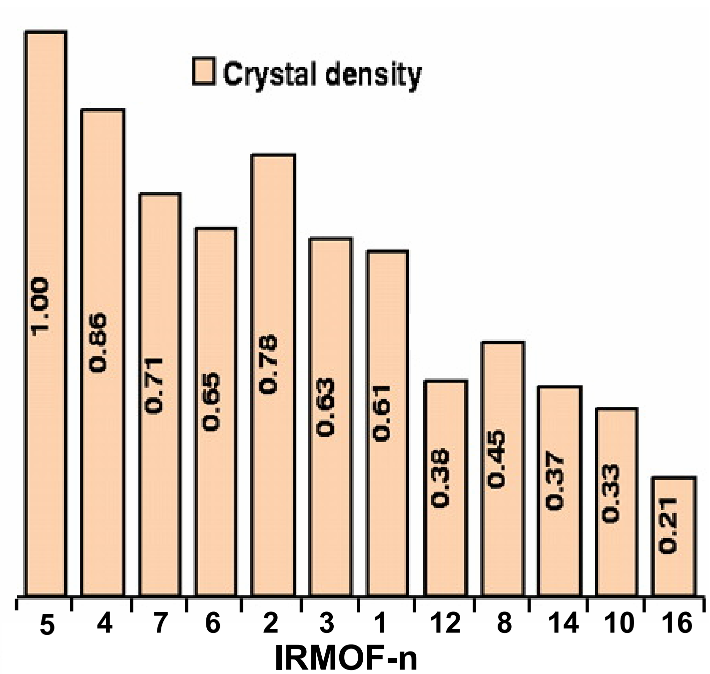


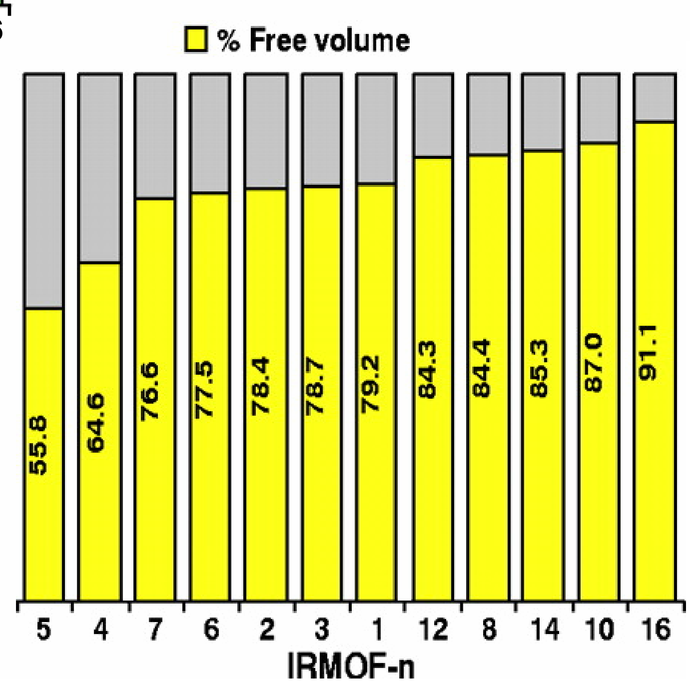
Synthesis of an Isoreticular Series of MOFs



Variation in MOF Metrical Parameters





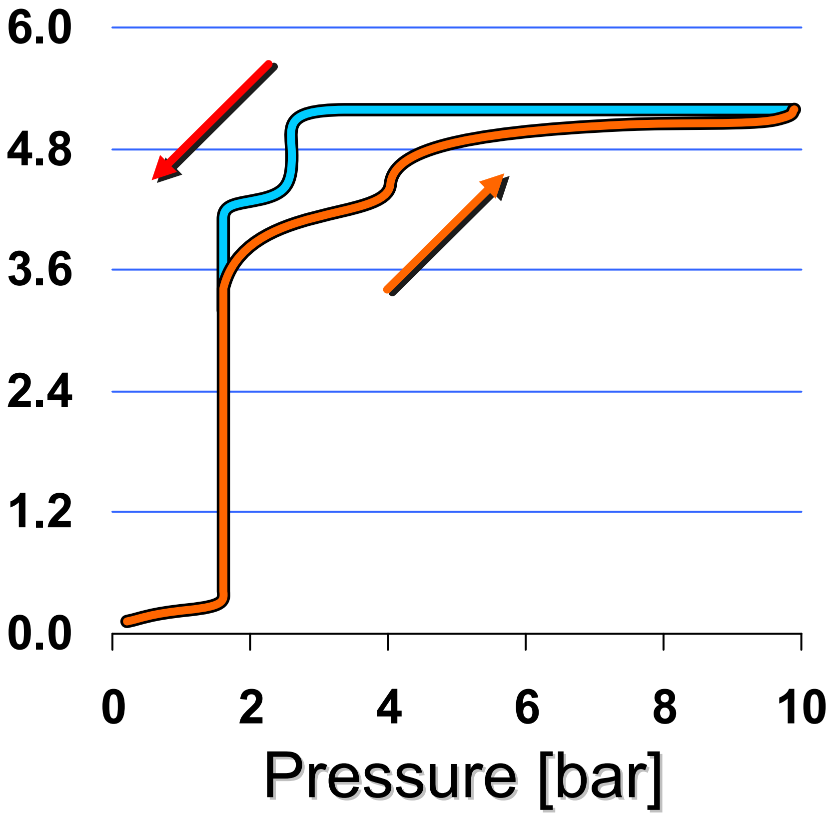


Mechanism of H_2 Uptake in MOFs

Chemisorption

Mg-Hydride, 300 °C

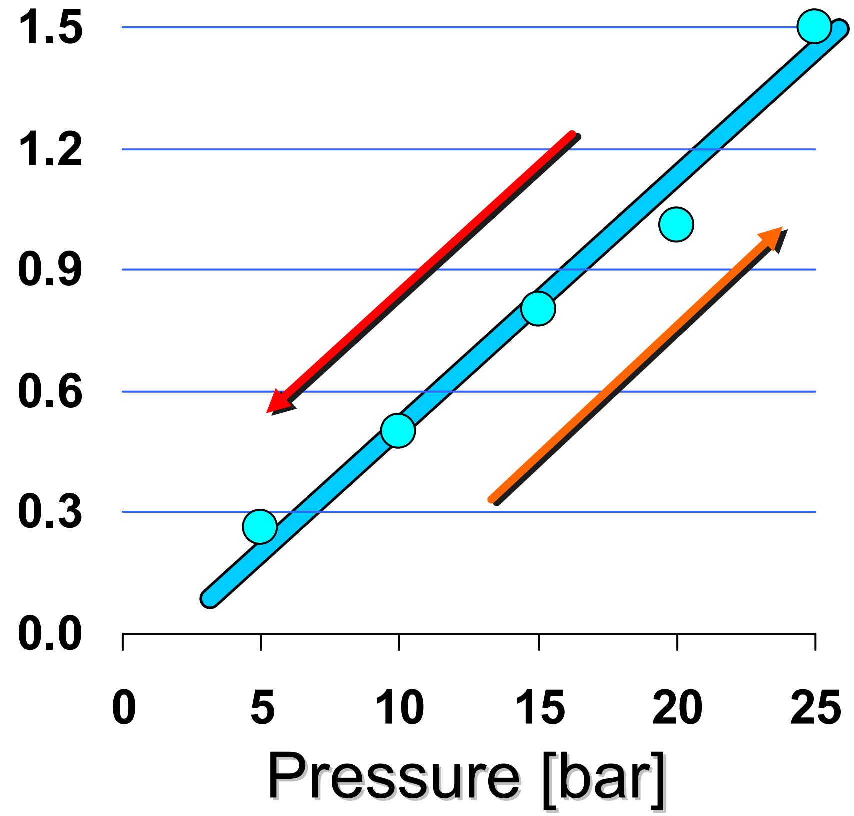
Weight % H_2



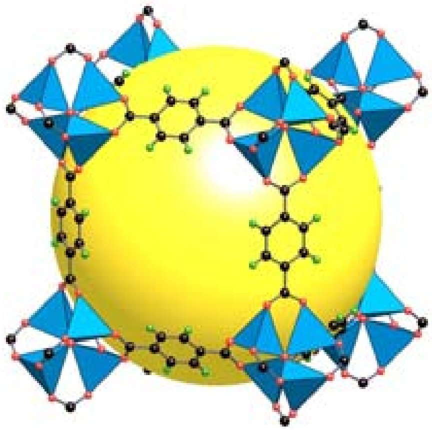
Physisorption

MOF-5, 24 °C

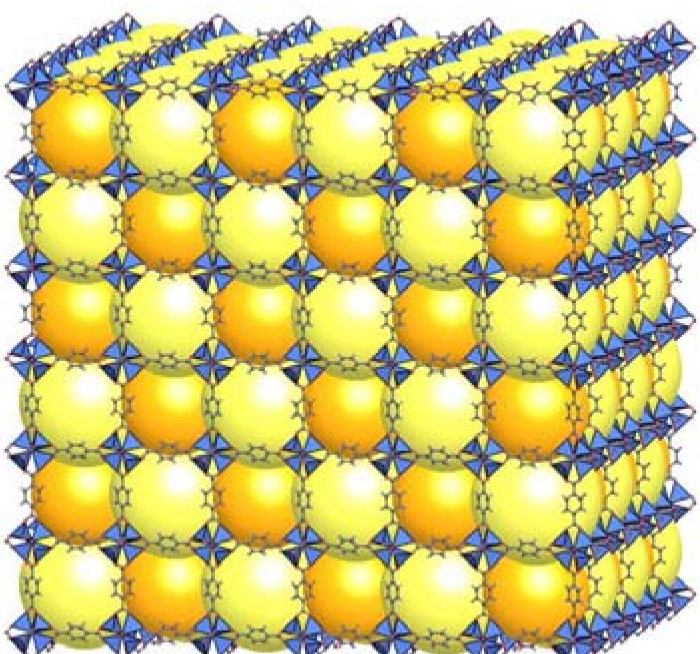
Weight % H_2



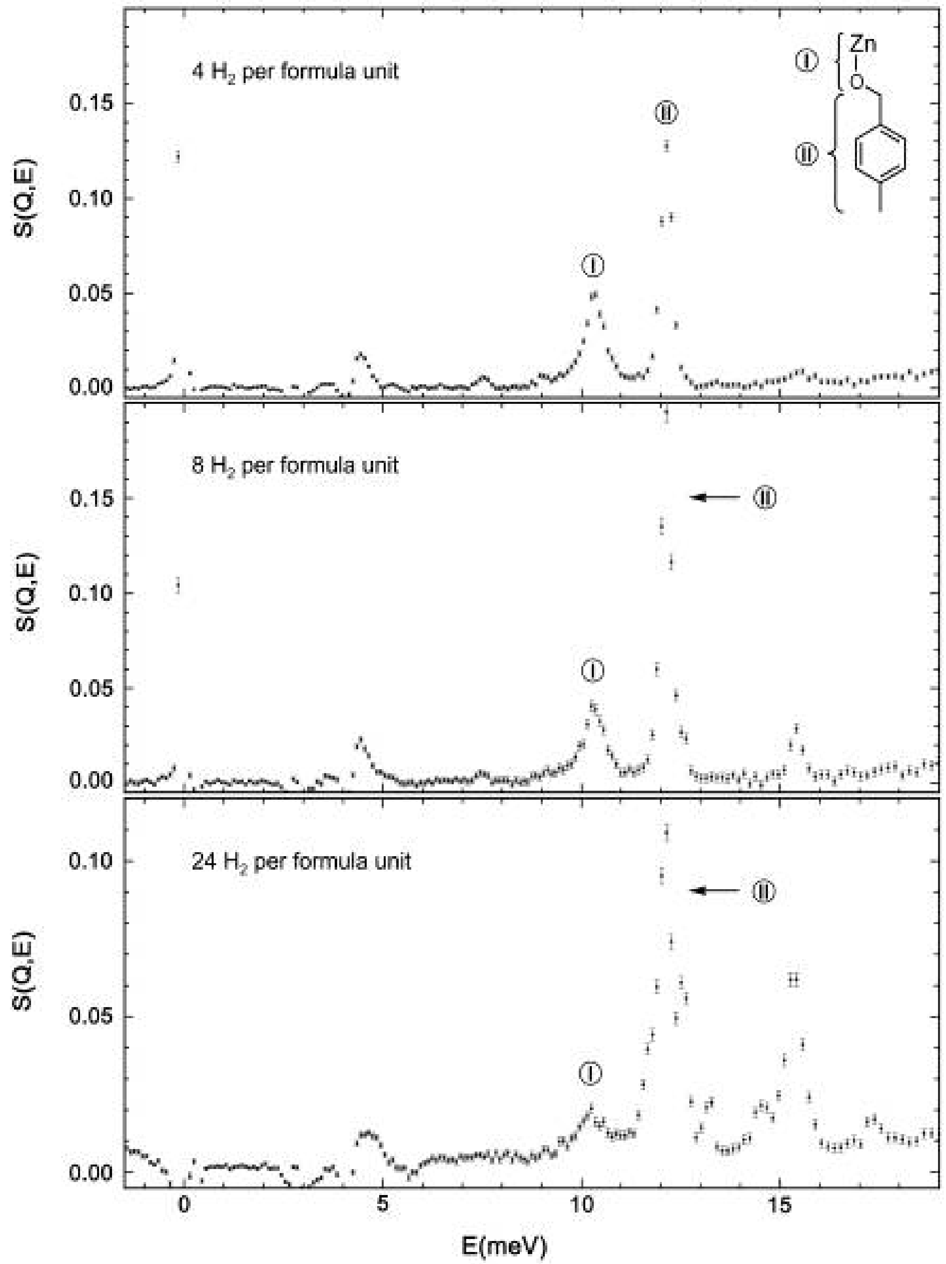
Inelastic Neutron Scattering of H_2 in MOF-5



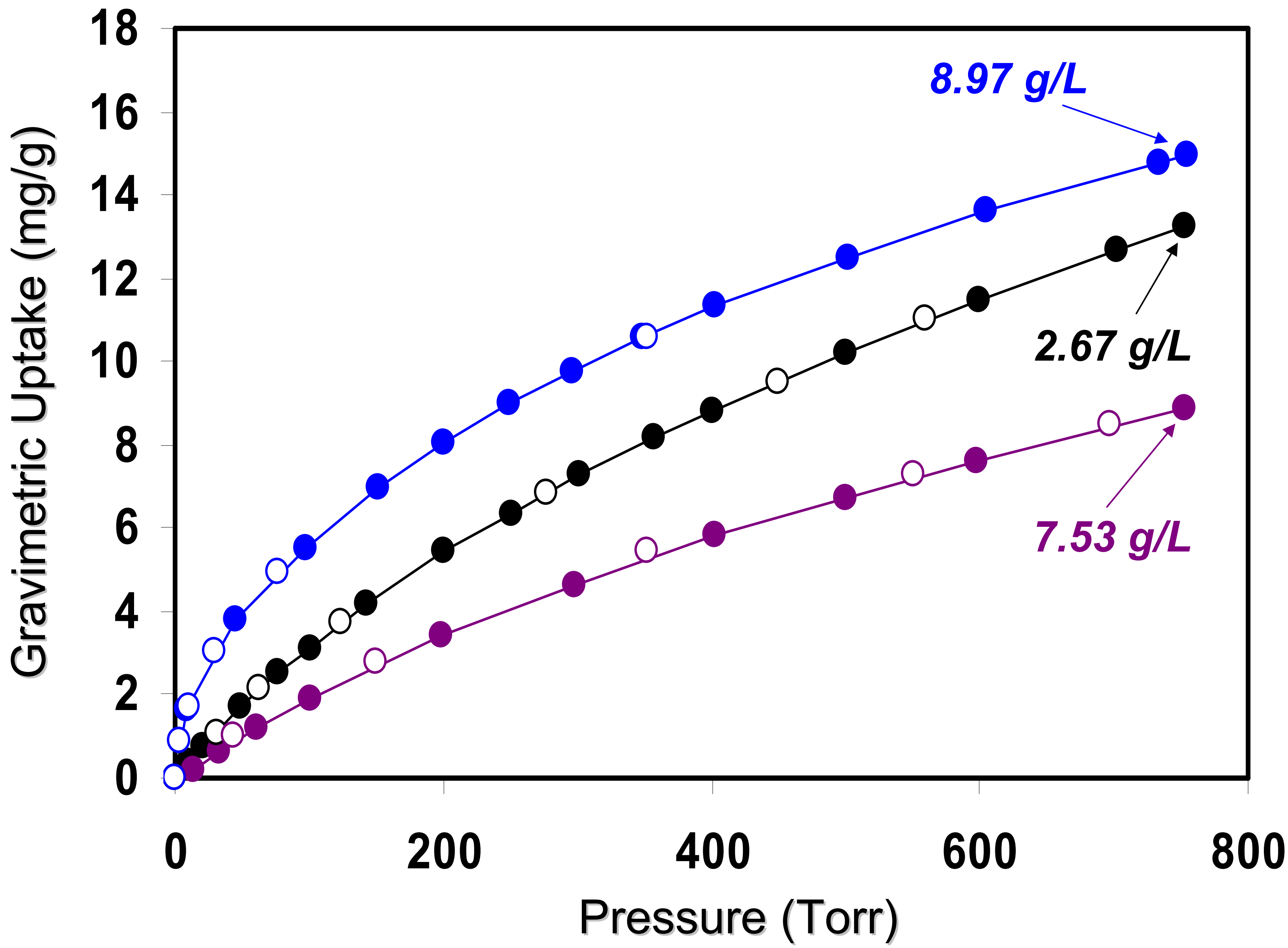
Smallest repeat unit of MOF-5



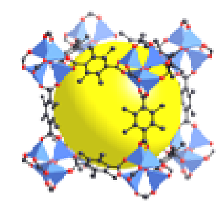
Extended structure of MOF-5



H_2 Sorption at 1 atm & 77 K



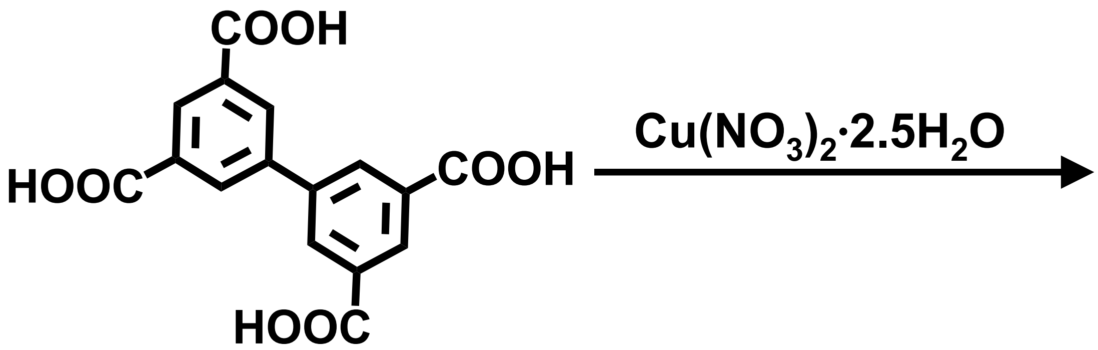
IRMOF-1



IRMOF-18

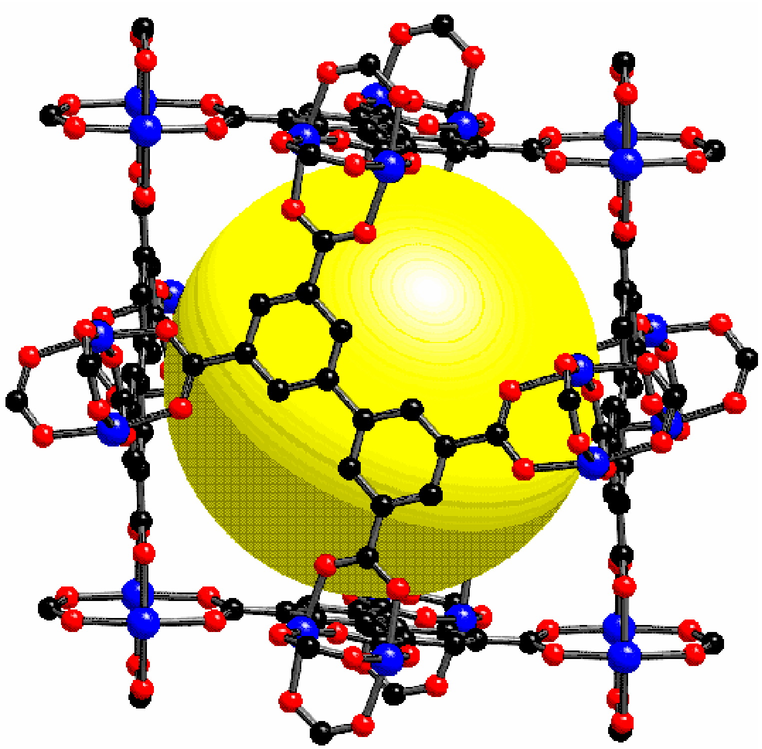
IRMOF-8

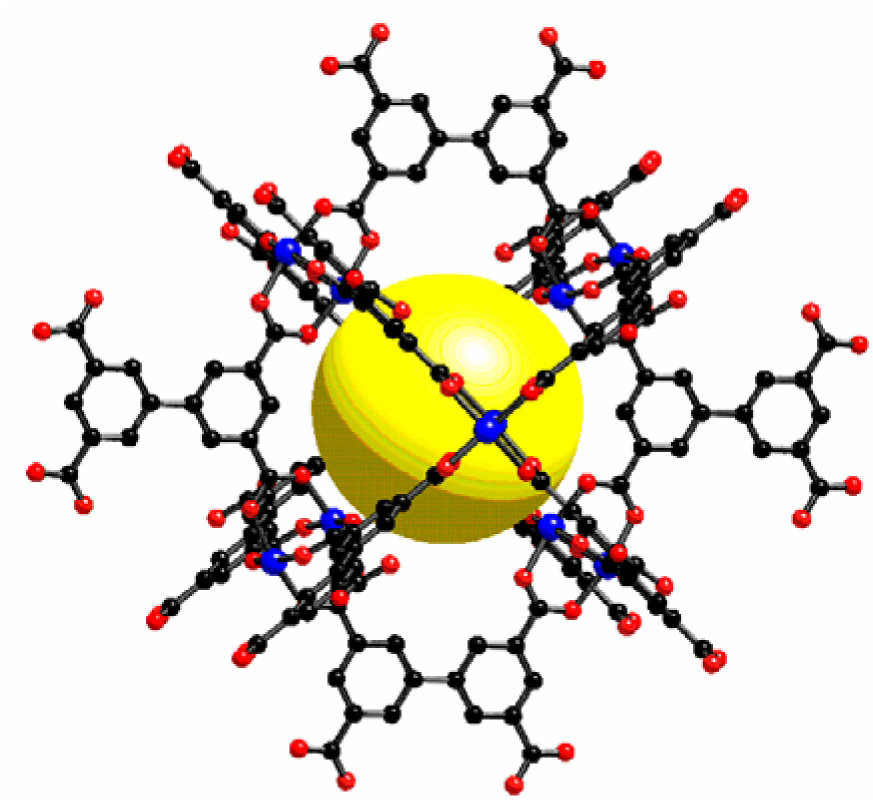
Synthesis of a Cu-based MOF



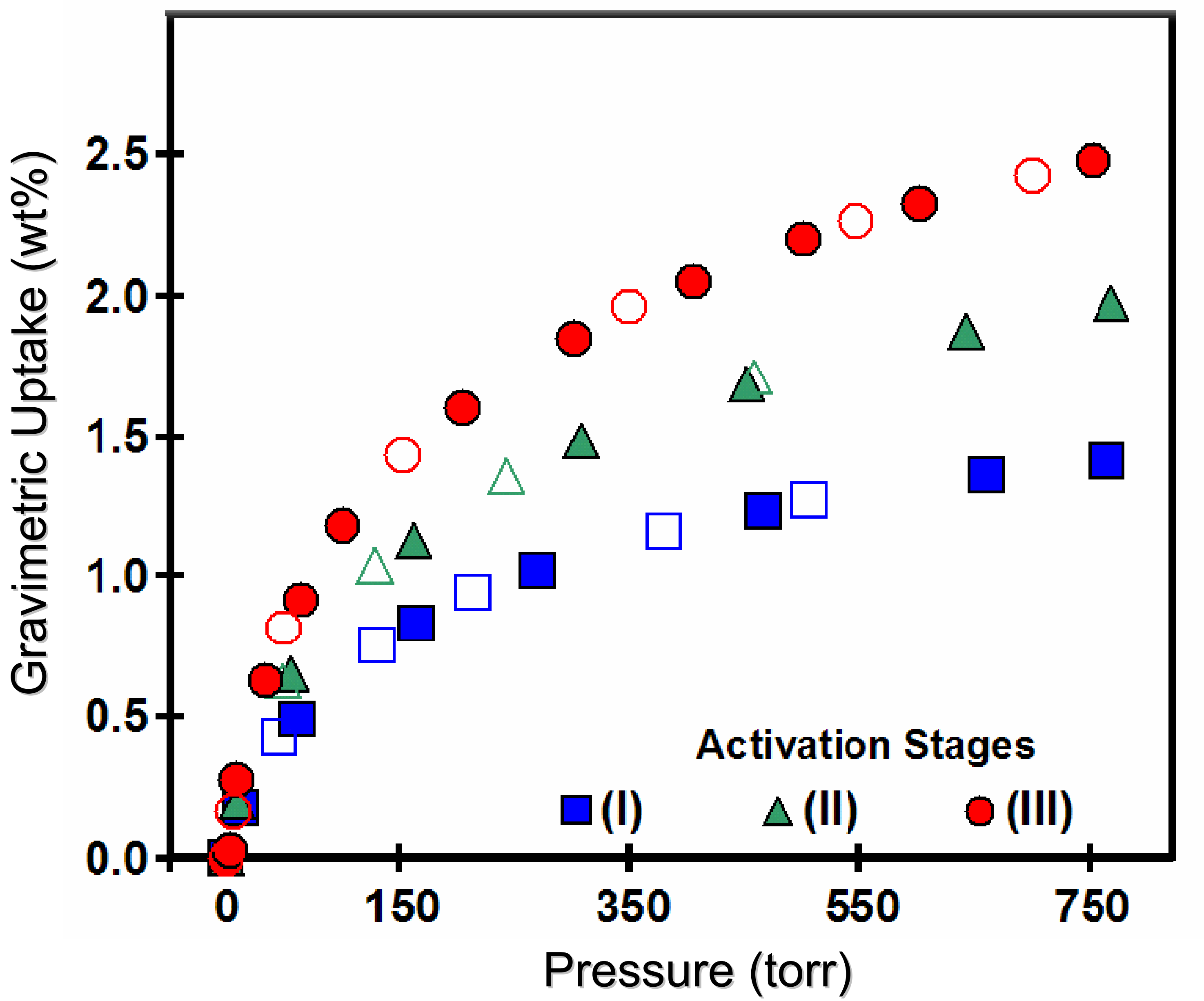
$Cu_2(BPTC)(H_2O)_2 \cdot (DMF)_3(H_2O)$

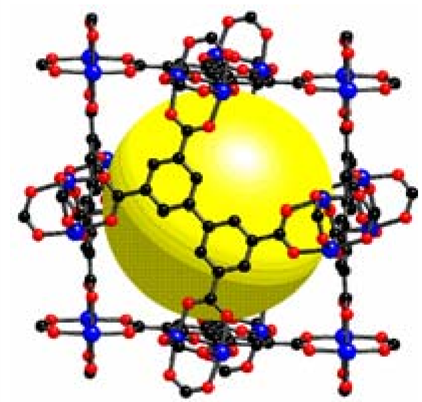
MOF-505





MOF-505 H_2 (77 K) Sorption Isotherms– Activation Study





MOF-505

Future Work

TASK	2005	2006	2007	2008	2009
Task 1: Equilibrium H_2 Uptake vs Structure		Go/ No-go Option	Go/ No-go Option		
Measure temperature and pressure dependence of H_2 uptake in 4 existing MOFs					
Computational design of new linkers					
Explore new linkers					
Task 2: Thermodynamics & Kinetics H_2 Uptake					
Determine H_2 binding energy to framework by sorption					
Analysis H_2 uptake rates in single crystals by Raman spectroscopy					
Measure H_2 flux in single x-tals					
Task 3: Mechanism of H_2 Uptake					
Analysis H_2 binding sites in MOFs by Raman spectroscopy					
NMR measurement of H_2 uptake					
Task 4: Down-select Optimum Materials					
Optimize scale-up synthesis and activation					
Cost analysis of material					

Publications and Presentations

Please list any publications and presentations that have resulted from work on this project.

- *No publications resulting from current funding at this stage of the project.*

Hydrogen Safety

The most significant hydrogen hazard associated with this project is:

- High exposure to H_2 gas with possibility of personal injury due to decreased oxygen content in the atmosphere.
- High concentrations of H_2 may pose a fire or explosion in and around instrumentation.

Hydrogen Safety

Our approach to deal with this hazard:

- Dedicated a single laboratory for all H_2 experiments.
- Installed active ventilation snorkles from laboratory hoods to all instrumentation consuming/ releasing H_2.
- Installed atmospheric H_2 detector (ppm level detection) outfitted with an alarm in the dedicated laboratory.

Acknowledgements