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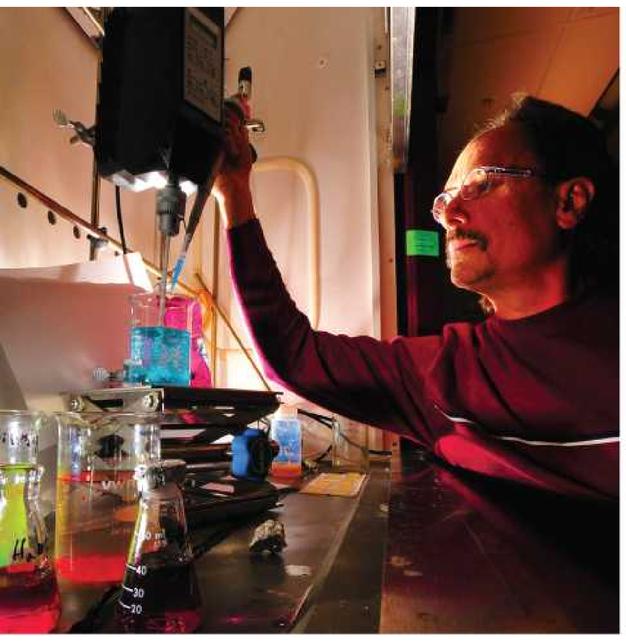

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SAND No. 2011-XXXXP

Stability and Endurance of Metal-Organic Frameworks Under Applications-Based Pressure Extremes

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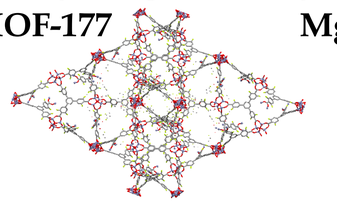
Abstract

The challenge of safe hydrogen gas storage has proven to be a major roadblock in developing clean, renewable hydrogen-fueled vehicles. Metal-organic frameworks (MOFs) are a class of highly porous crystalline materials that are attractive for their promising hydrogen gas adsorption capabilities, potentially enabling the storage of large amounts of hydrogen gas in compact tanks under moderate pressures. With real-world applications in mind, we examine MOF stability under realistic pressure conditions in the hydrogen fuel tank of a car.

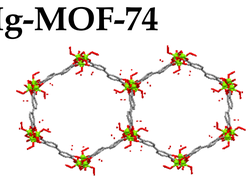
Project Goals

1. Determine stability and endurance of a variety of characteristic MOFs under pressure cycling
2. Offer insight into which MOF characteristics impact stability under pressure cycling and why

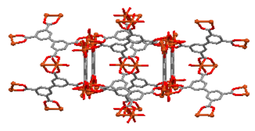
MOF-177



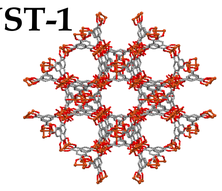
Mg-MOF-74



NOTT-100



HKUST-1



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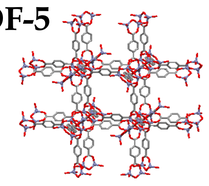

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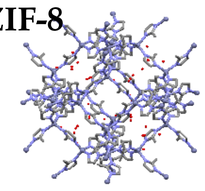
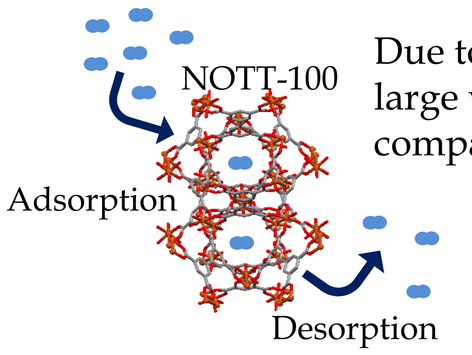


Hydrogen Storage



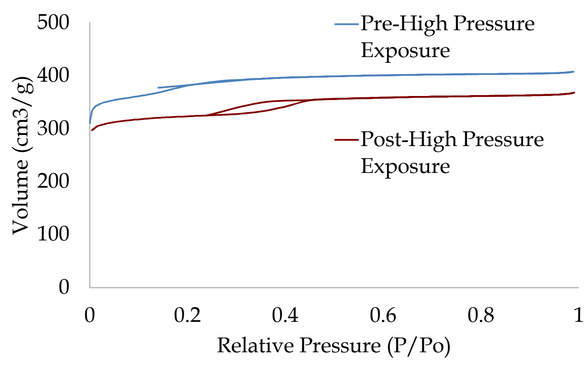
Due to the ultra-high porosity of many MOFs, large volumes of hydrogen gas can be stored compactly in MOF pores via **physisorption**

While adsorption and desorption of gases at low pressures is reversible in MOFs, exposure to high pressures over time (700 bar for 25 hr) appears to damage some MOFs more than others, shifting nitrogen isotherm plots and lowering surface areas:.

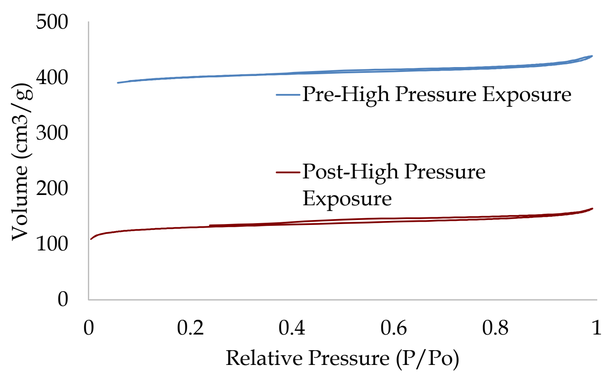
NOTT-100 ΔBET SA: **223 cm²/g**
Mg-MOF-74 Δ BET SA: **885 cm²/g**

In order to meet DOE targets, MOFs will need to withstand extensive pressure cycling of 5-100 bar over the course of a vehicle's lifetime.

NOTT-100, Pre and Post 700 bar (25 hr)



Mg-MOF-74, Pre and Post 700 bar (25 hr)



Measuring MOF Stability

1. Synthesize MOFs

● + Metal Organic Linker

Solvothermal syntheses encourage slow crystal growth, ensuring high phase purity

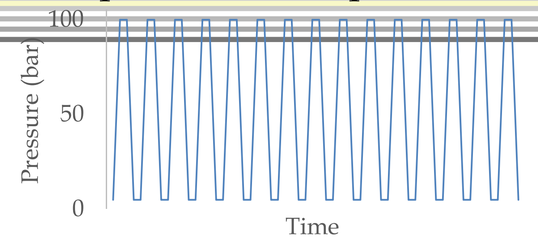
2. Characterize guest-free MOFs

Activated MOFs undergo a series of characterization measurements:

- H_2 and N_2 isotherms
  - Surface Area
  - Pore Volume
- Powder XRD
- Raman
- FTIR

3. Pressure Cycling

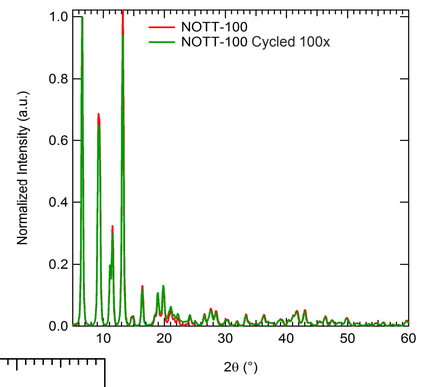
To simulate realistic refueling and consumption cycles in the hydrogen fuel tank of a vehicle, MOFs are exposed to 1,000 pressure cycles of 5-100 bar H_2



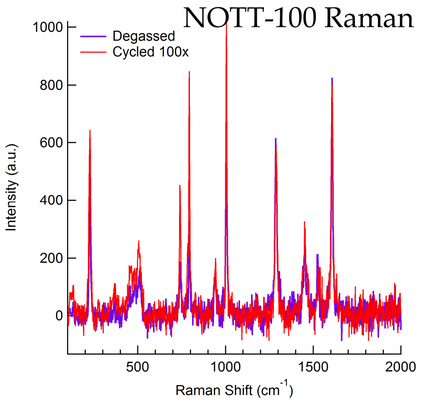
4. Characterize & Compare

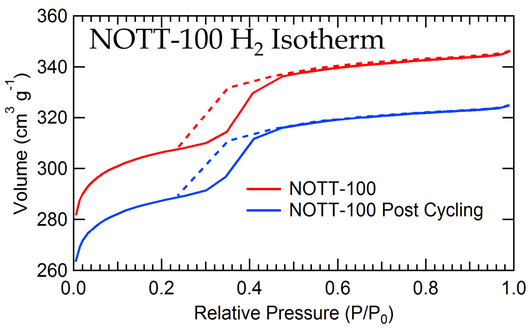
The cycled MOFs undergo identical characterization measurements from pre-cycling in order to quantitatively analyze their stability

NOTT-100 PXRD



NOTT-100 Raman





Pre-cycling BET SA: **1080 m²/g**
Post-cycling BET SA: **1067 m²/g**

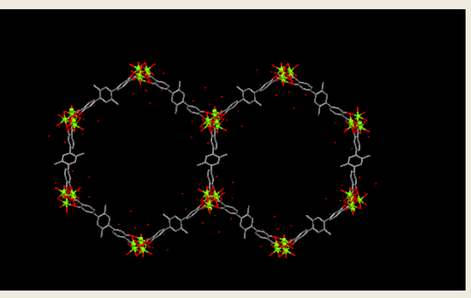
While the chemical structure, crystallinity, and surface area remain constant, there appears to be a minor 6% decrease in hydrogen adsorption capability

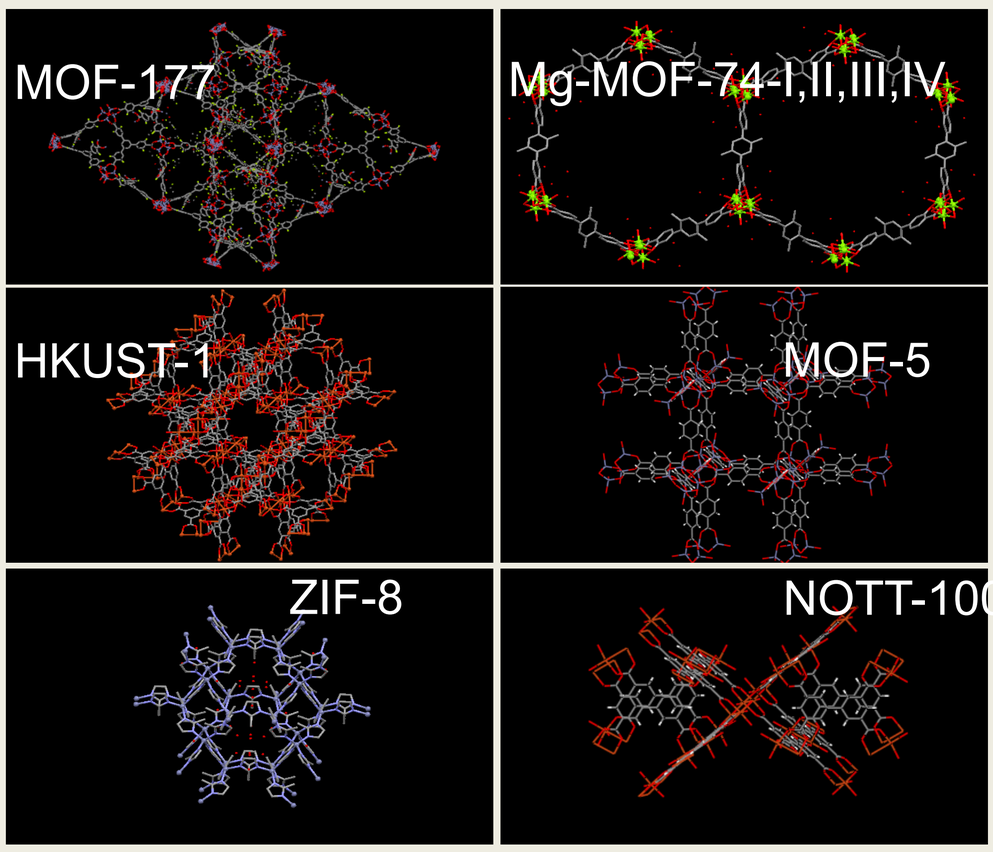
Results and Future Work

While it is clear that extensive high pressure exposure damages some MOFs, it is unclear to what extent moderate pressure cycling reduces hydrogen MOF adsorption capabilities, if at all. The chosen array of characteristics MOFs must undergo pressure cycling and analysis in to understand if and how MOFs are impacted. This work will allow future researchers to gain a stronger understanding of the reversibility of hydrogen adsorption in MOFs and help identify candidate MOFs for hydrogen storage in vehicles.

Acknowledgments

Special thanks to James White for his prior work and immense help on the project. This work was funded by the Hydrogen Materials Advanced Research Consortium as part of the Energy Materials Network, under the U.S. Department of Energy's Clean Energy Manufacturing Initiative.

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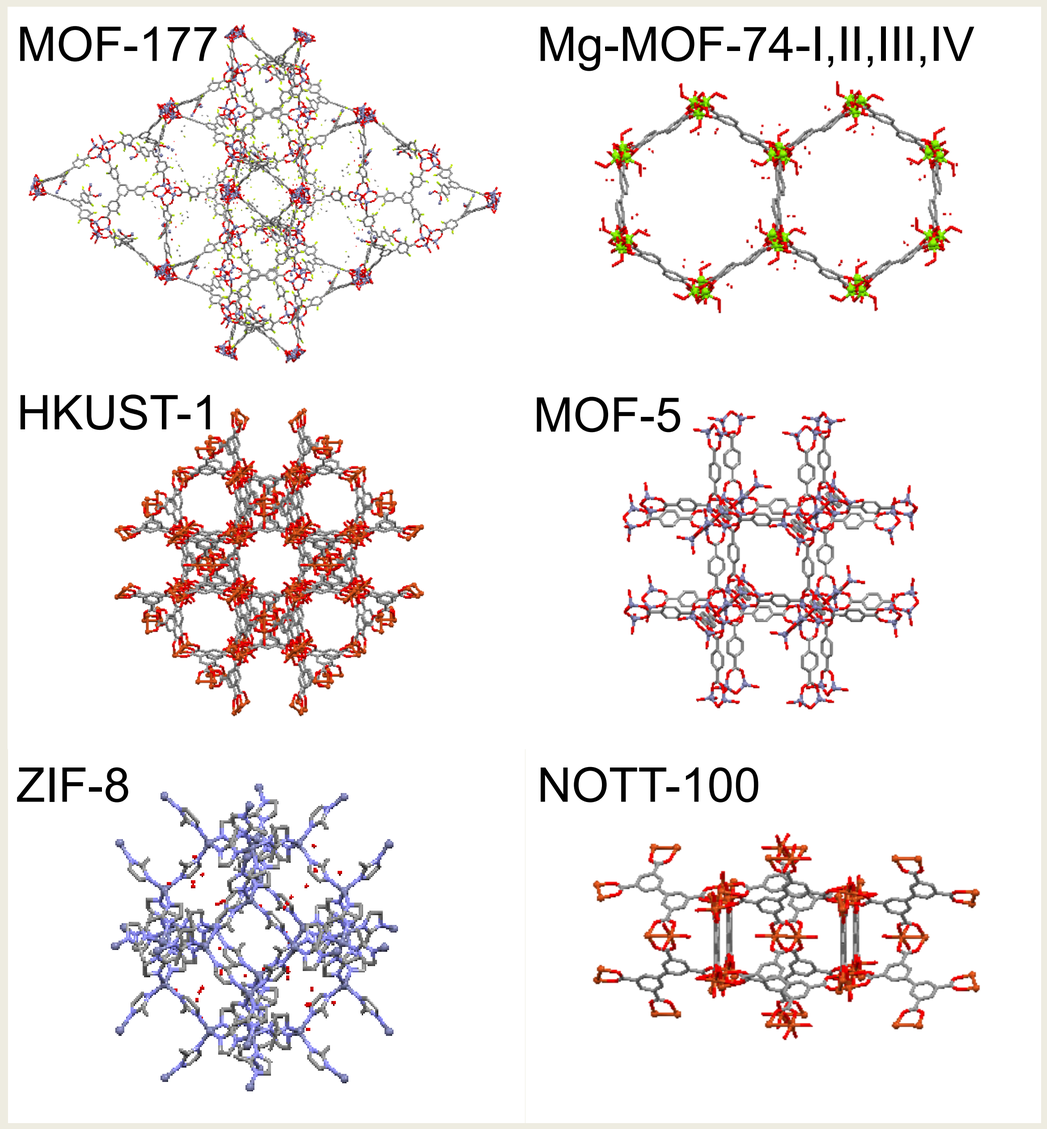
Mg-MOF-74-I,II,III,IV
HKUST-1
MOF-5
ZIF-8
NOTT-100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