

High-Throughput Methodology for Discovery of Metal-Organic Frameworks with a High Hydrogen Binding Enthalpy

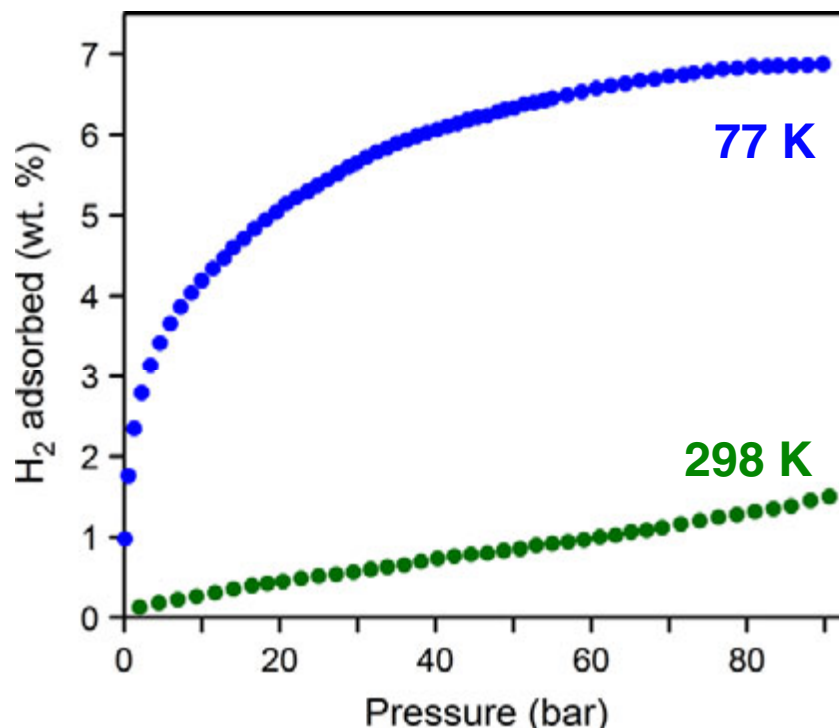
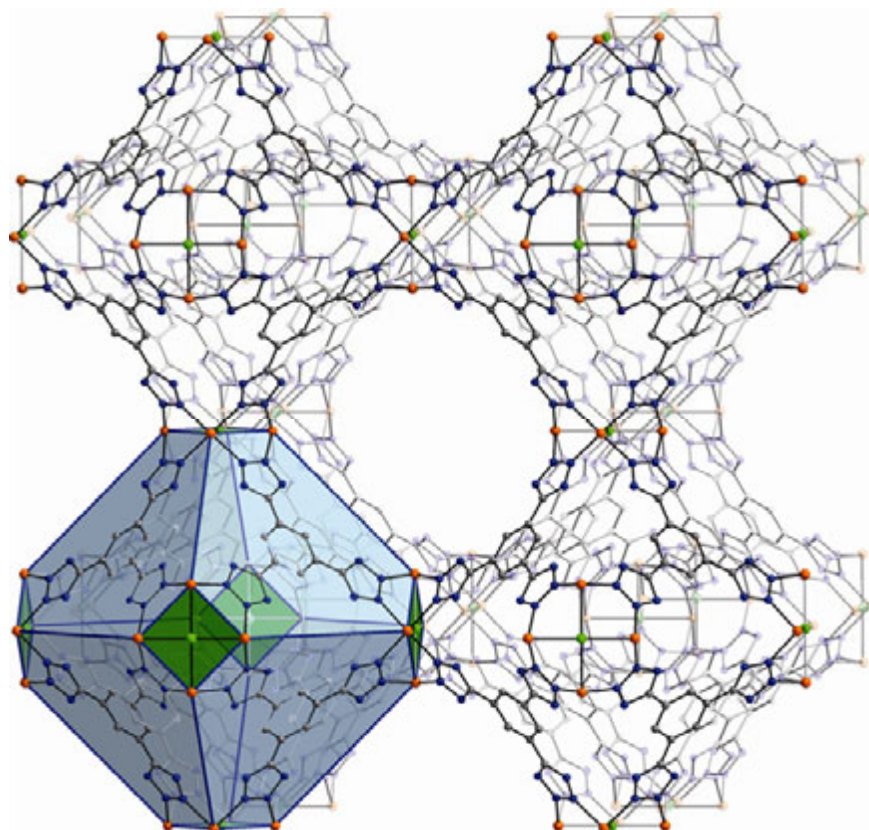
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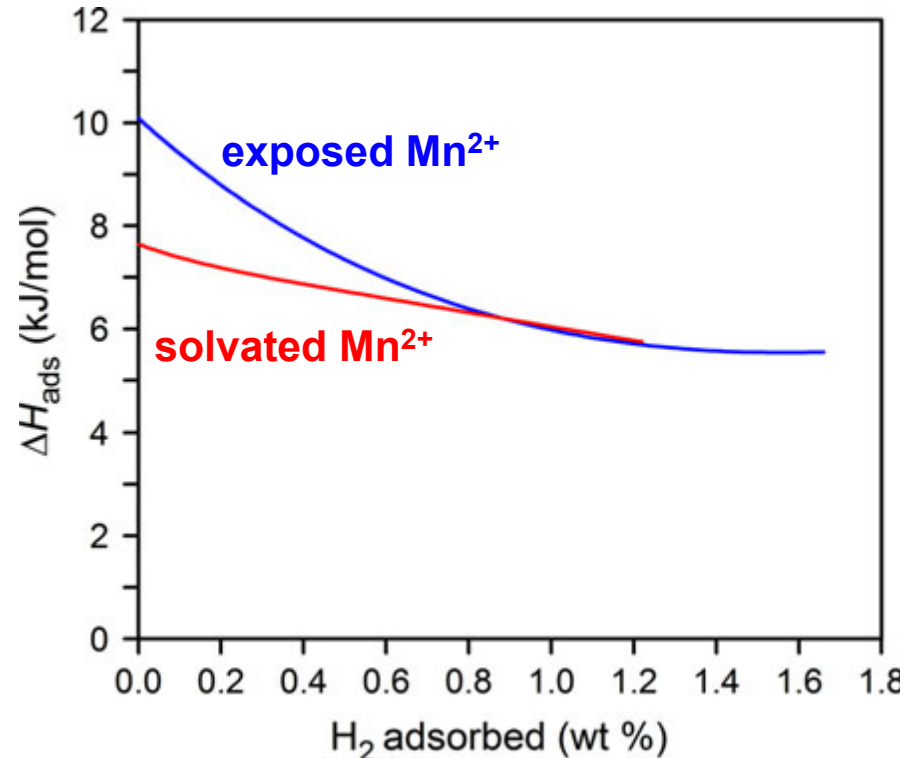
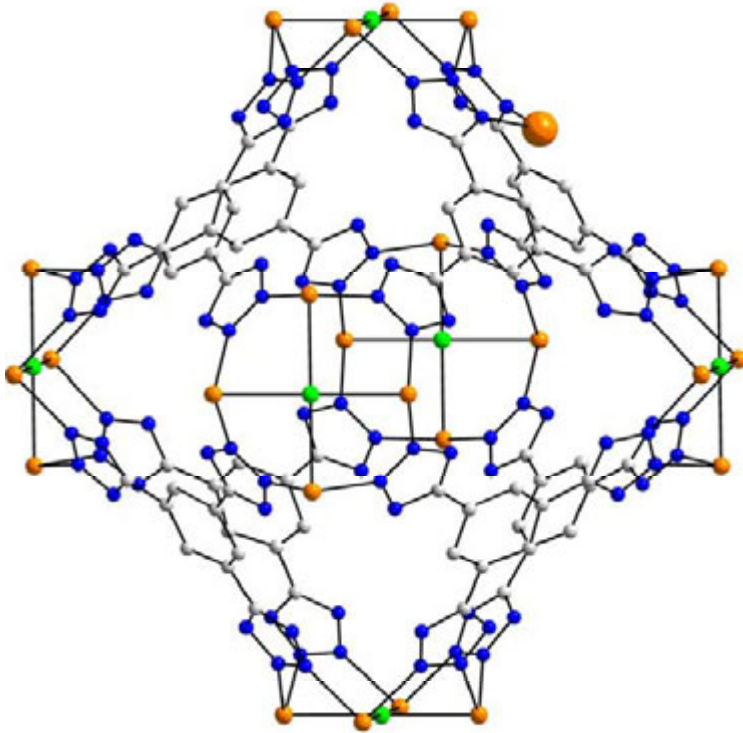
Symyx Technologies, Inc.

A Tetrazolate-Bridged Framework with Exposed Mn^{2+} Sites



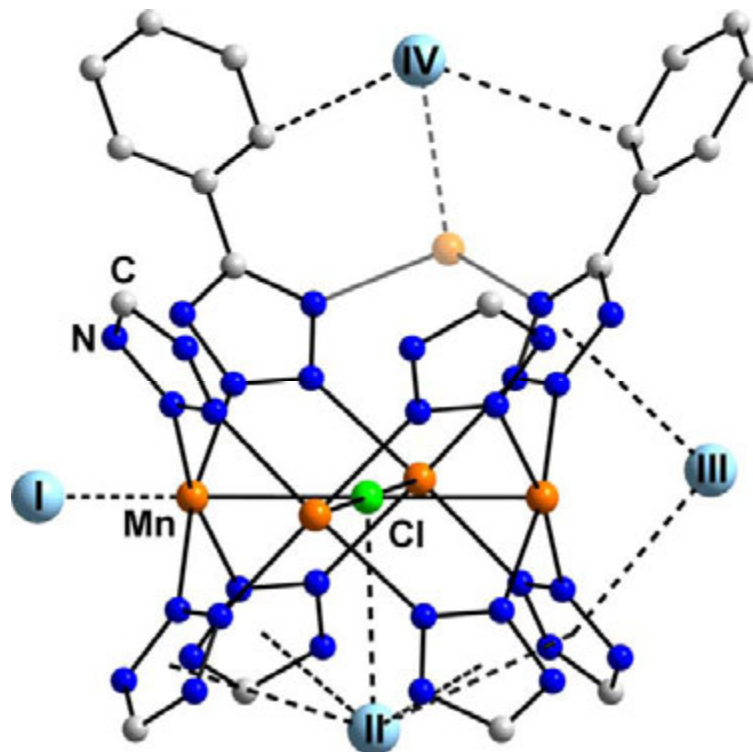
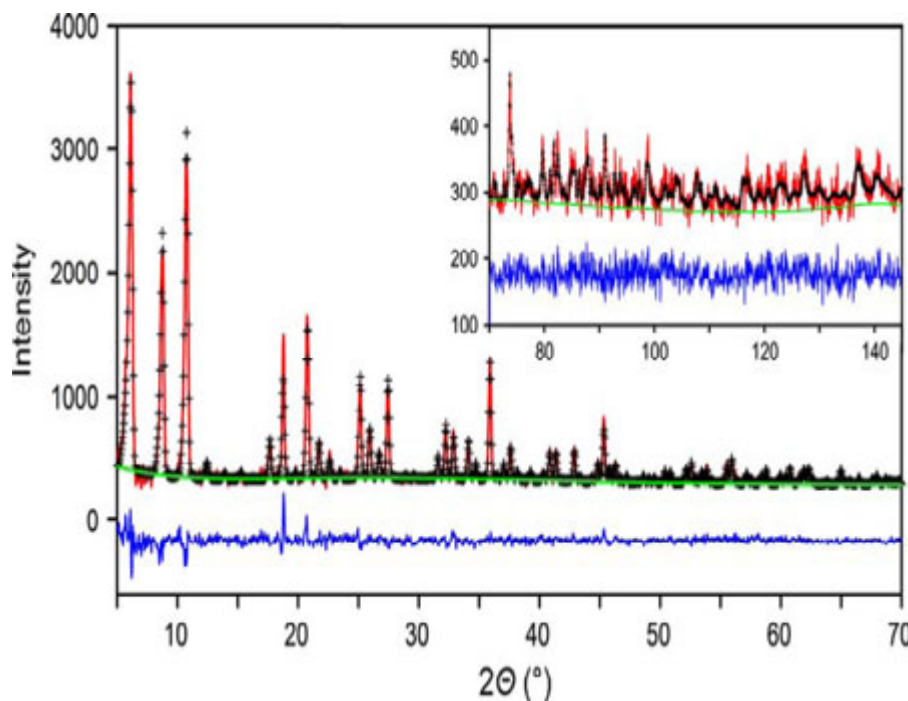
- Volumetric storage at 90 bar and 77 K is **60 g/L** (85% density of liquid H_2 at 21 K)
- Volumetric storage at 90 bar and 298 K is 50% greater than in an empty cylinder

Increased H₂ Adsorption Enthalpy at Exposed Metals



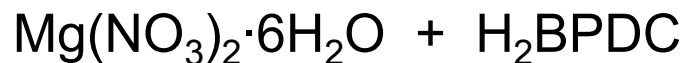
- Binding enthalpies at low loading are now as high as 10 kJ/mol
- Exposed Mn²⁺ coordination sites are only a small weight fraction of available sites
- Attempts to replace Mn²⁺ with stronger-binding cations (e.g. Cu⁺) are underway

Locating D₂ Adsorption Sites by Neutron Diffraction



- Strongest D₂ binding occurs at sites I (Mn-D₂ = 2.2 Å) and II (Cl...D₂ = 3.5 Å)
- First direct observation of metal-D₂ interaction in a metal-organic framework

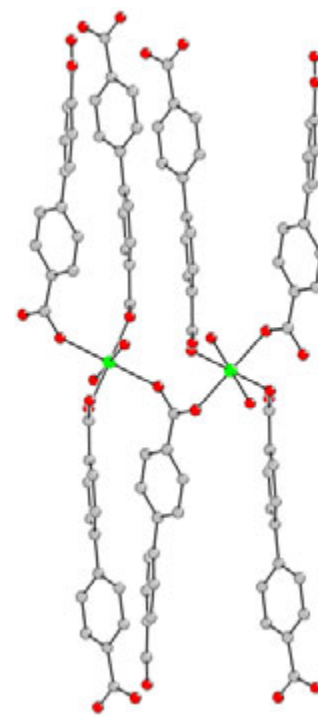
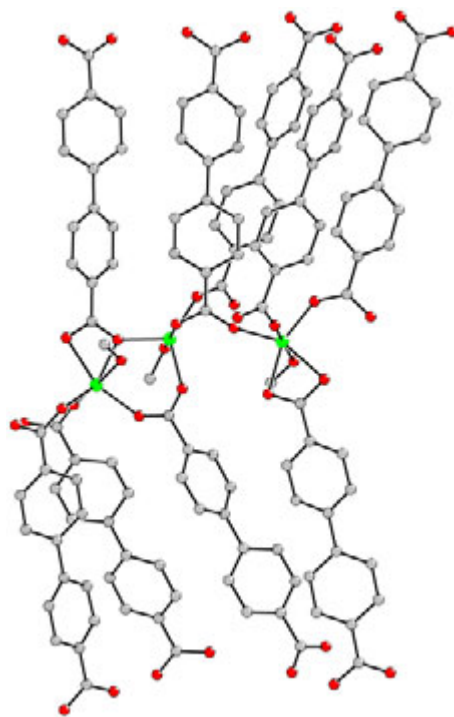
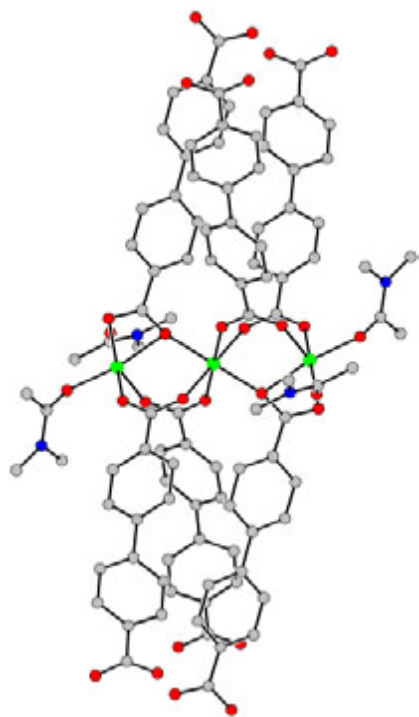
Synthesis Depends Critically on Reaction Conditions



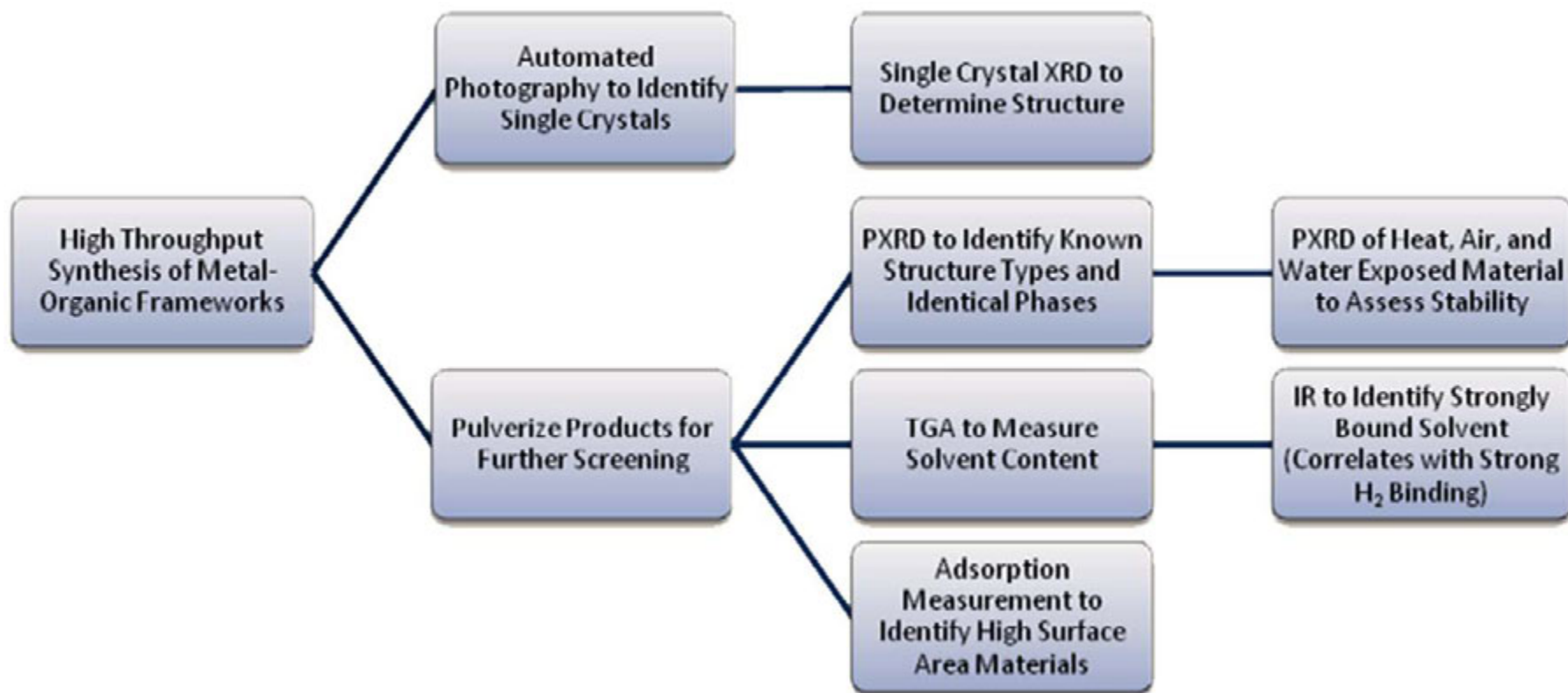
1% H_2O

2% H_2O

4% H_2O

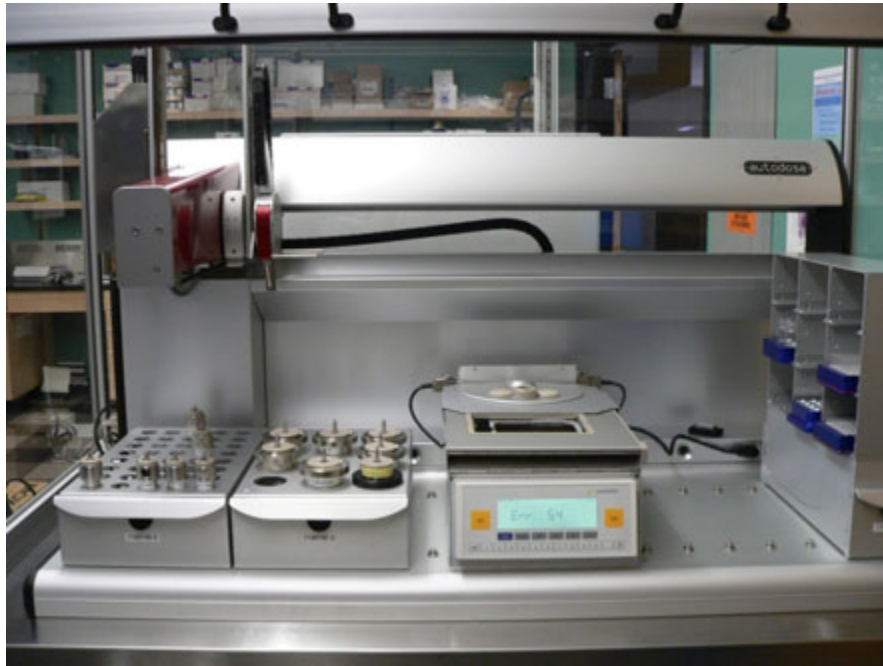


-Throughput Synthesis and Screening Process

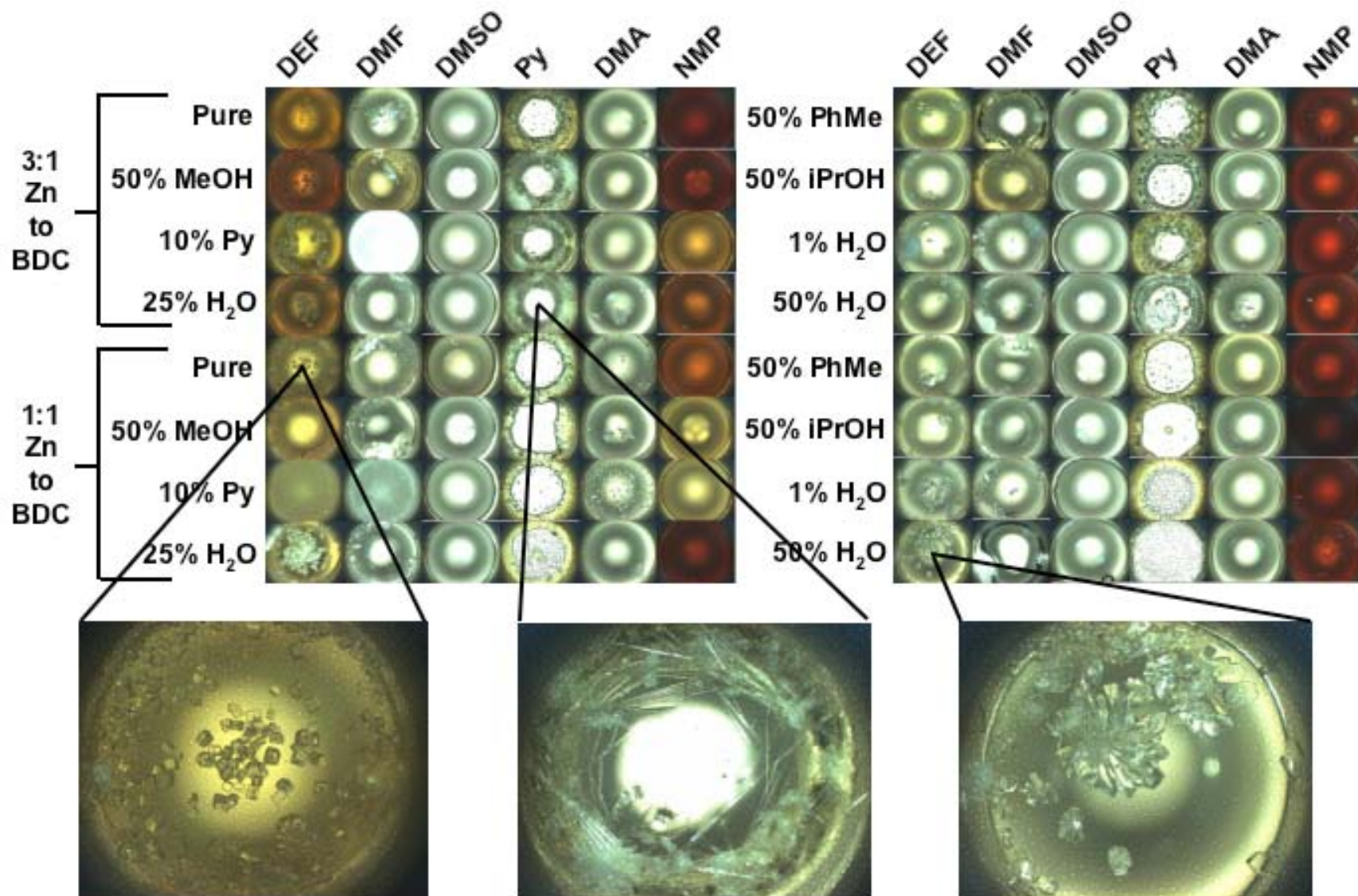


- Year 1: Develop reliable methods for high-throughput synthesis and screening
- Year 2: Utilize instrument for discovery of frameworks with exposed metal sites

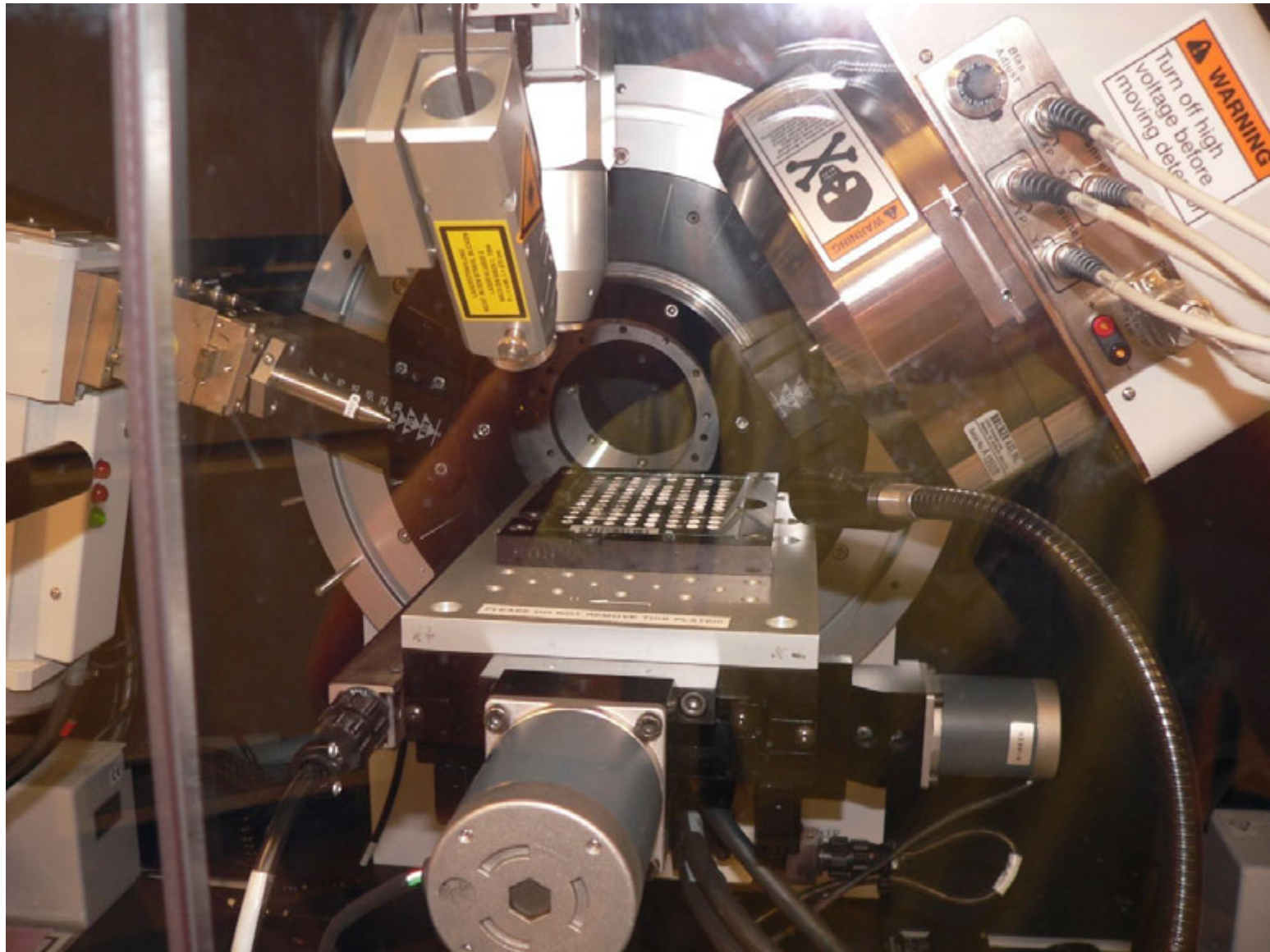
Core Modules for Solid and Liquid Handling



Test: $\text{Zn}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ + 1,4-Benzenedicarboxylic Acid



High-Throughput Powder X-Ray Diffraction



Satoshi Horike and Steven Kaye

