

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

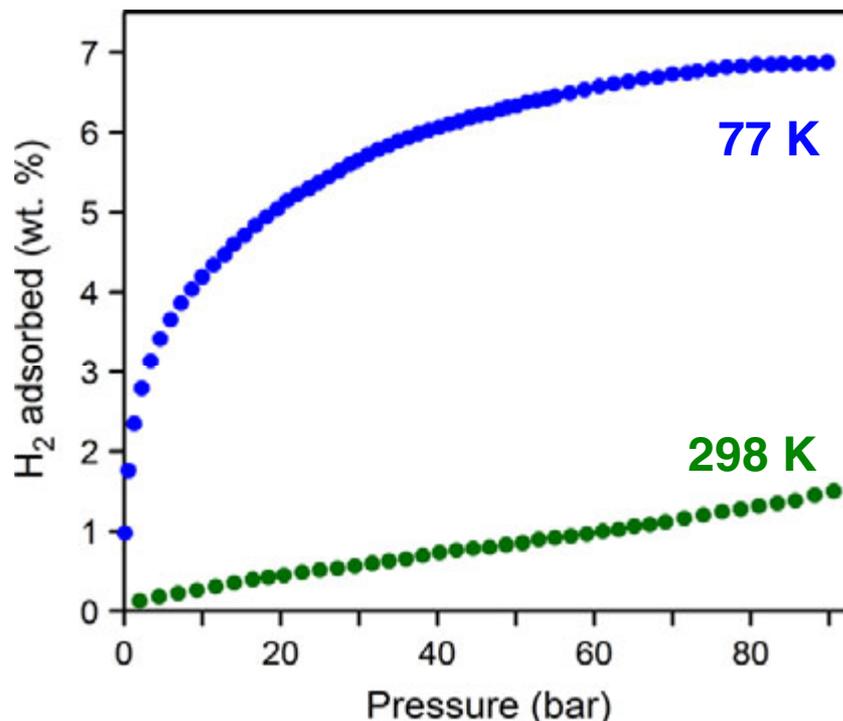
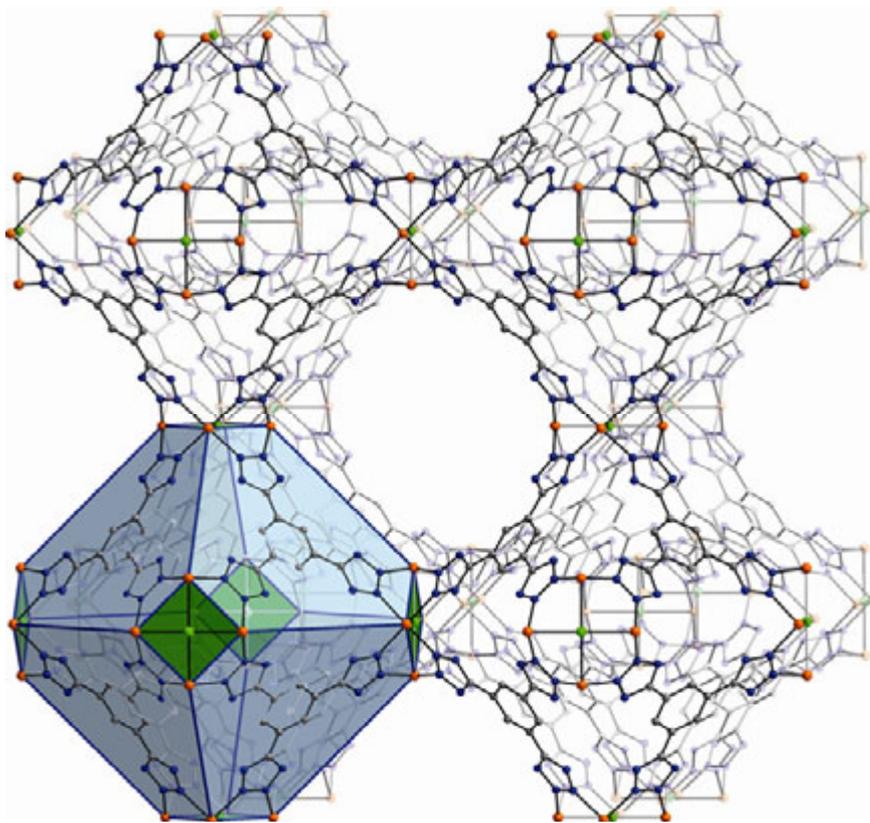
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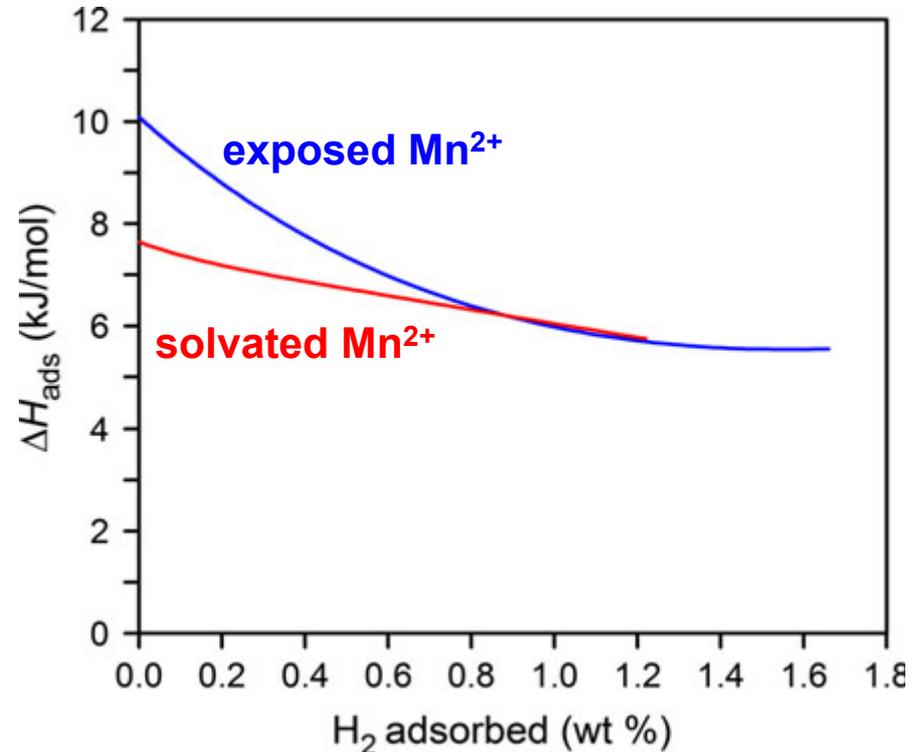
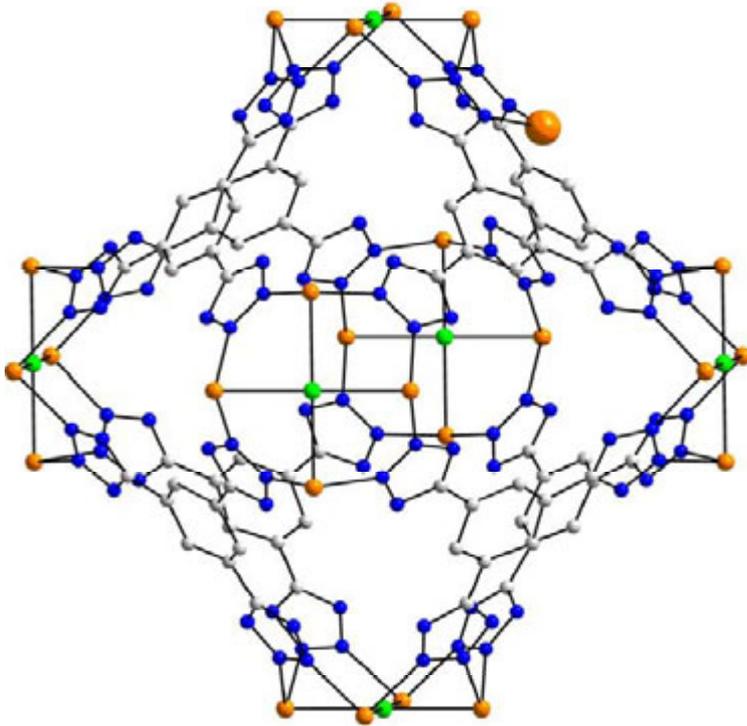
*Symyx Technologies, Inc.*

# A Tetrazolate-Bridged Framework with Exposed Mn<sup>2+</sup> Sites



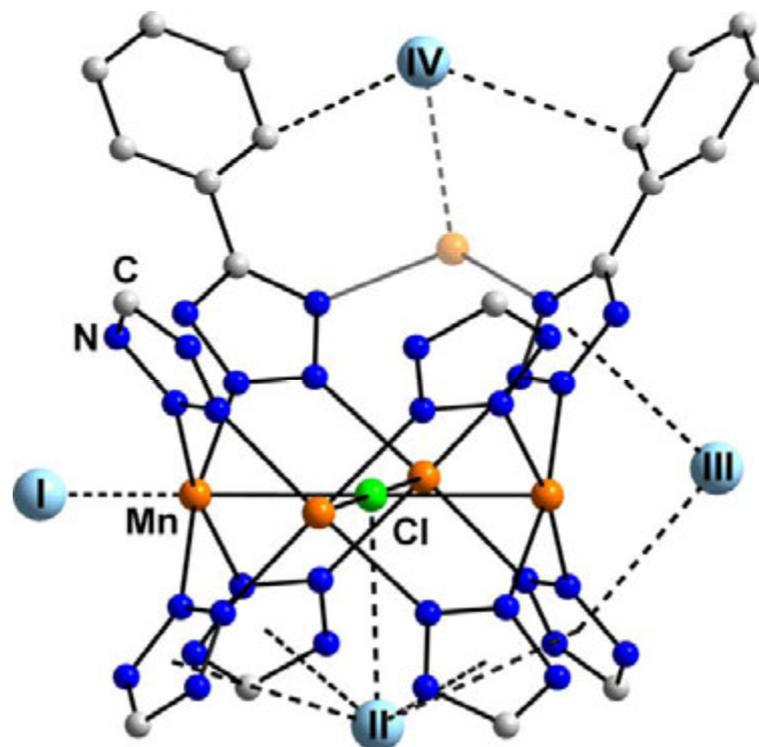
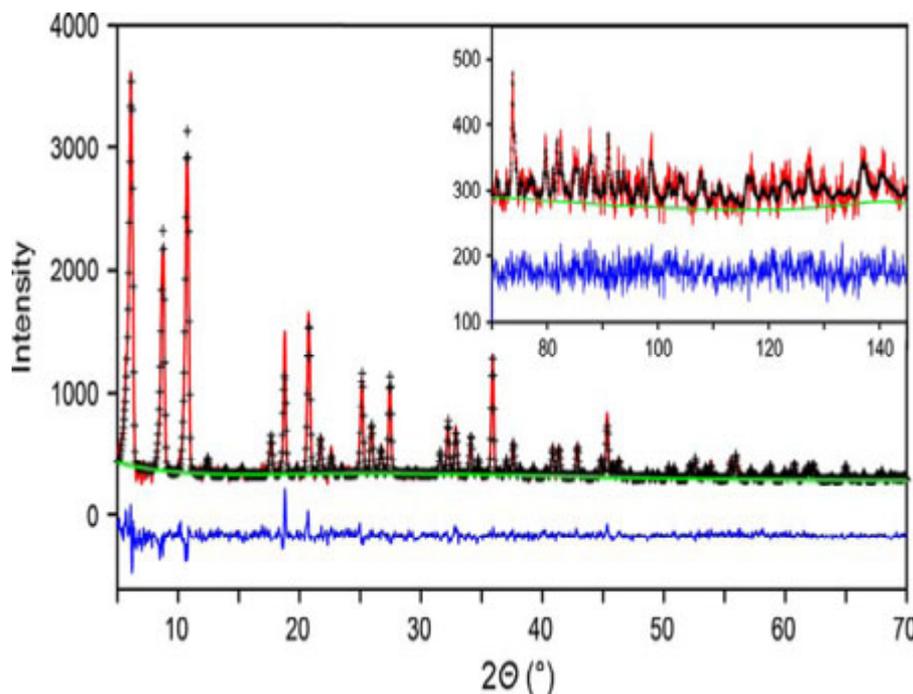
- Volumetric storage at 90 bar and 77 K is **60 g/L** (85% density of liquid H<sub>2</sub> at 21 K)
- Volumetric storage at 90 bar and 298 K is 50% greater than in an empty cylinder

# Increased H<sub>2</sub> Adsorption Enthalpy at Exposed Metals



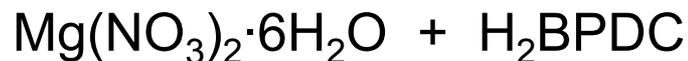
- Binding enthalpies at low loading are now as high as 10 kJ/mol
- Exposed Mn<sup>2+</sup> coordination sites are only a small weight fraction of available sites
- Attempts to replace Mn<sup>2+</sup> with stronger-binding cations (e.g. Cu<sup>+</sup>) are underway

# Locating D<sub>2</sub> Adsorption Sites by Neutron Diffraction



- Strongest D<sub>2</sub> binding occurs at sites I (Mn-D<sub>2</sub> = 2.2 Å) and II (Cl...D<sub>2</sub> = 3.5 Å)
- First direct observation of metal-D<sub>2</sub> interaction in a metal-organic framework

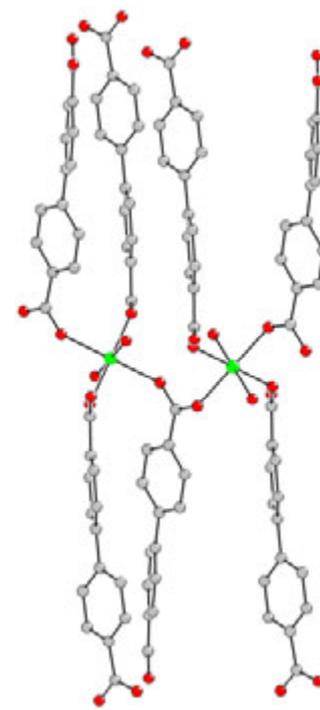
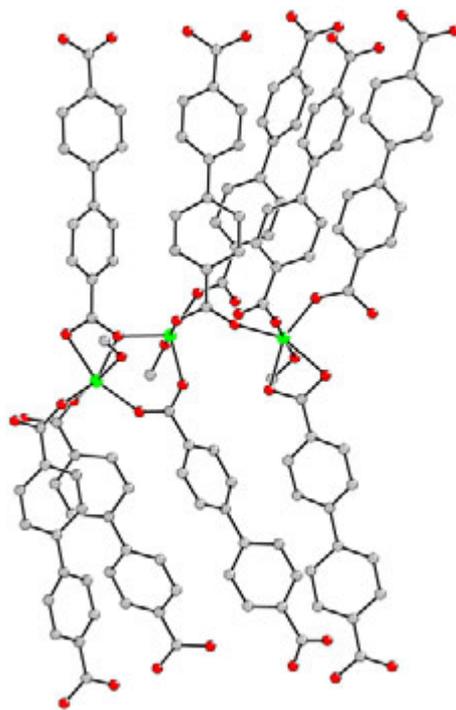
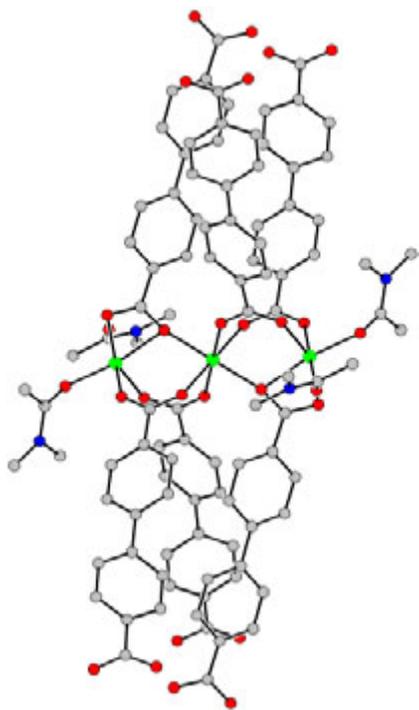
# Synthesis Depends Critically on Reaction Conditions



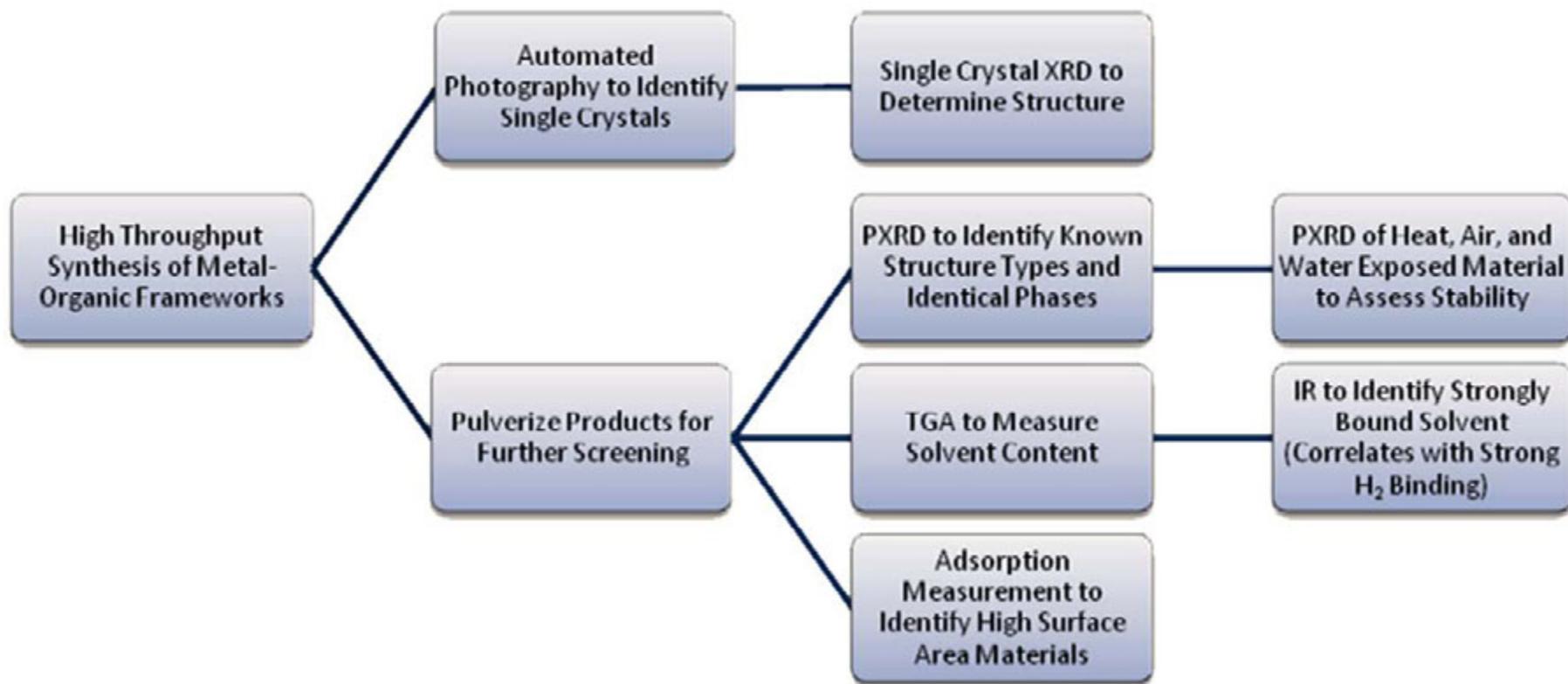
1% H<sub>2</sub>O

2% H<sub>2</sub>O

4% H<sub>2</sub>O



# -Throughput Synthesis and Screening Process

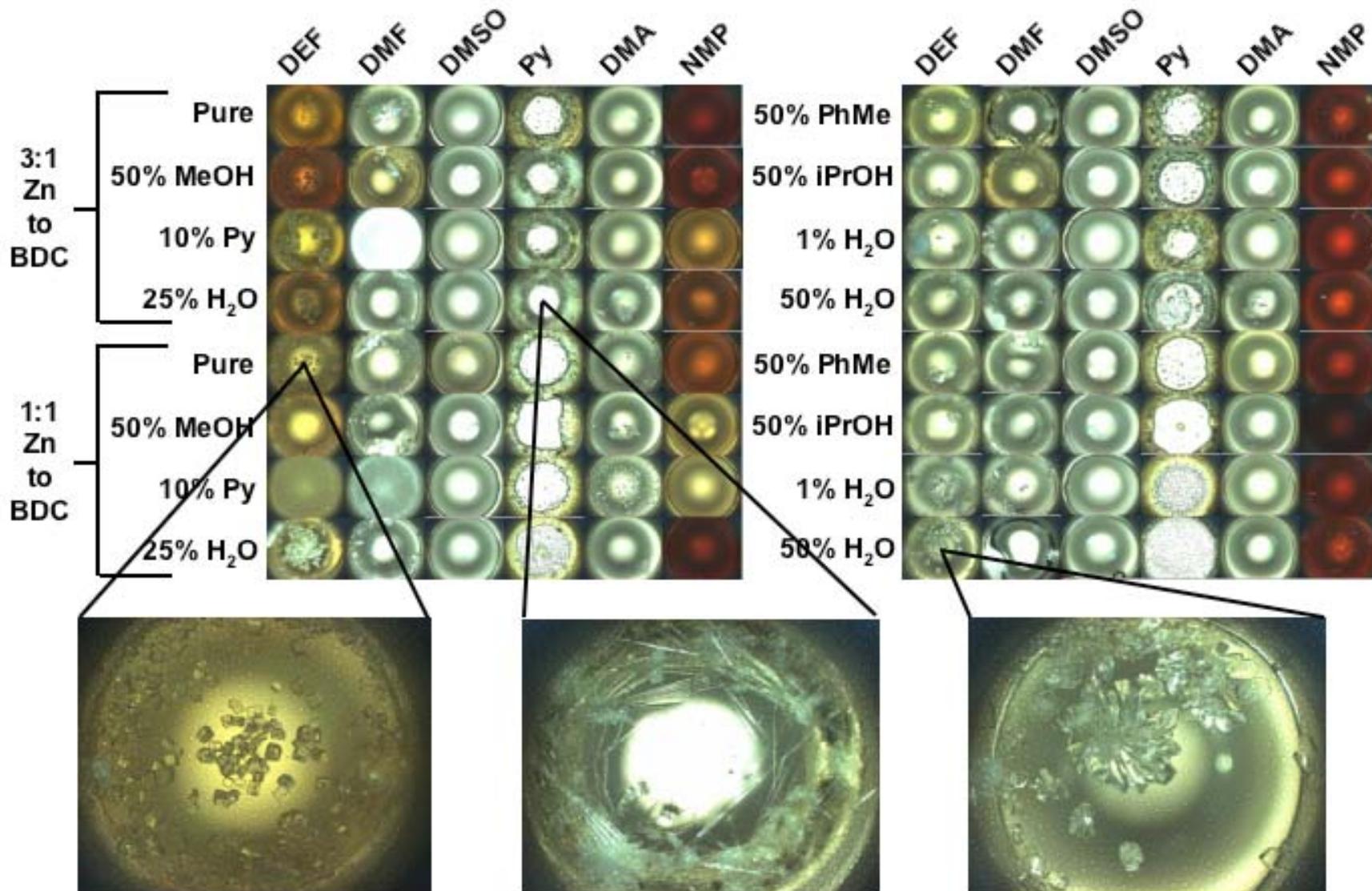


- Year 1: Develop reliable methods for high-throughput synthesis and screening
- Year 2: Utilize instrument for discovery of frameworks with exposed metal sites

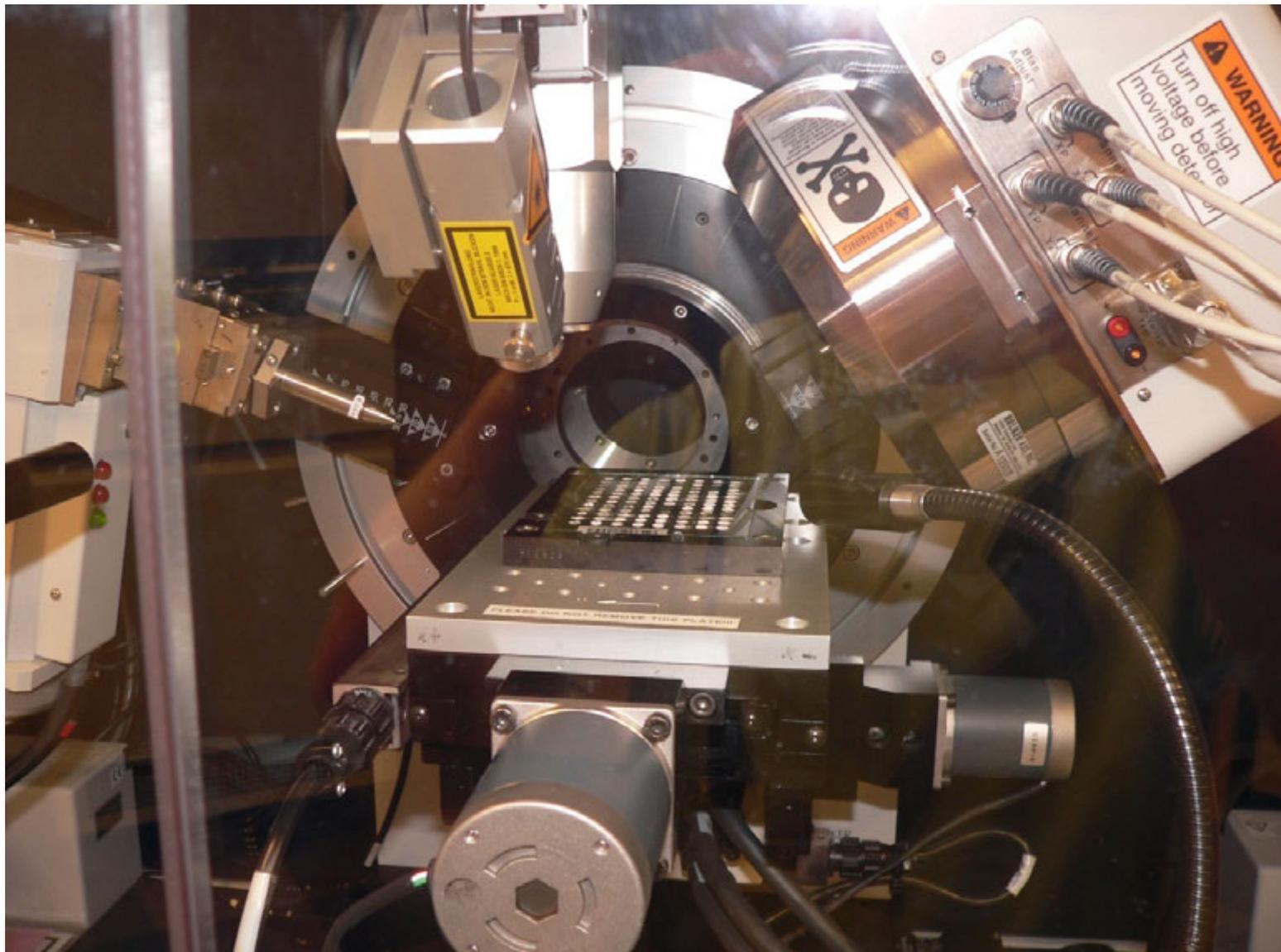
# Core Modules for Solid and Liquid Handling



# 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

