Characterizing Hydrogen Storage Materials Using Neutron Scattering Techniques

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Hydrogen Materials Advanced Research Consortium (HyMARC)
National Renewable Energy Laboratory
NIST Center for Neutron Research

About Me

Bachelors Degrees
Chemistry
Environmental Science

- Polypeptide complexes for advanced drug deliver systems

University of Chicago
2010 – 2014

Ph.D.
Inorganic Chemistry

- Emergent magnetism at high pressure
- Synthesis of new metastable perovskite materials using high pressure synthetic techniques

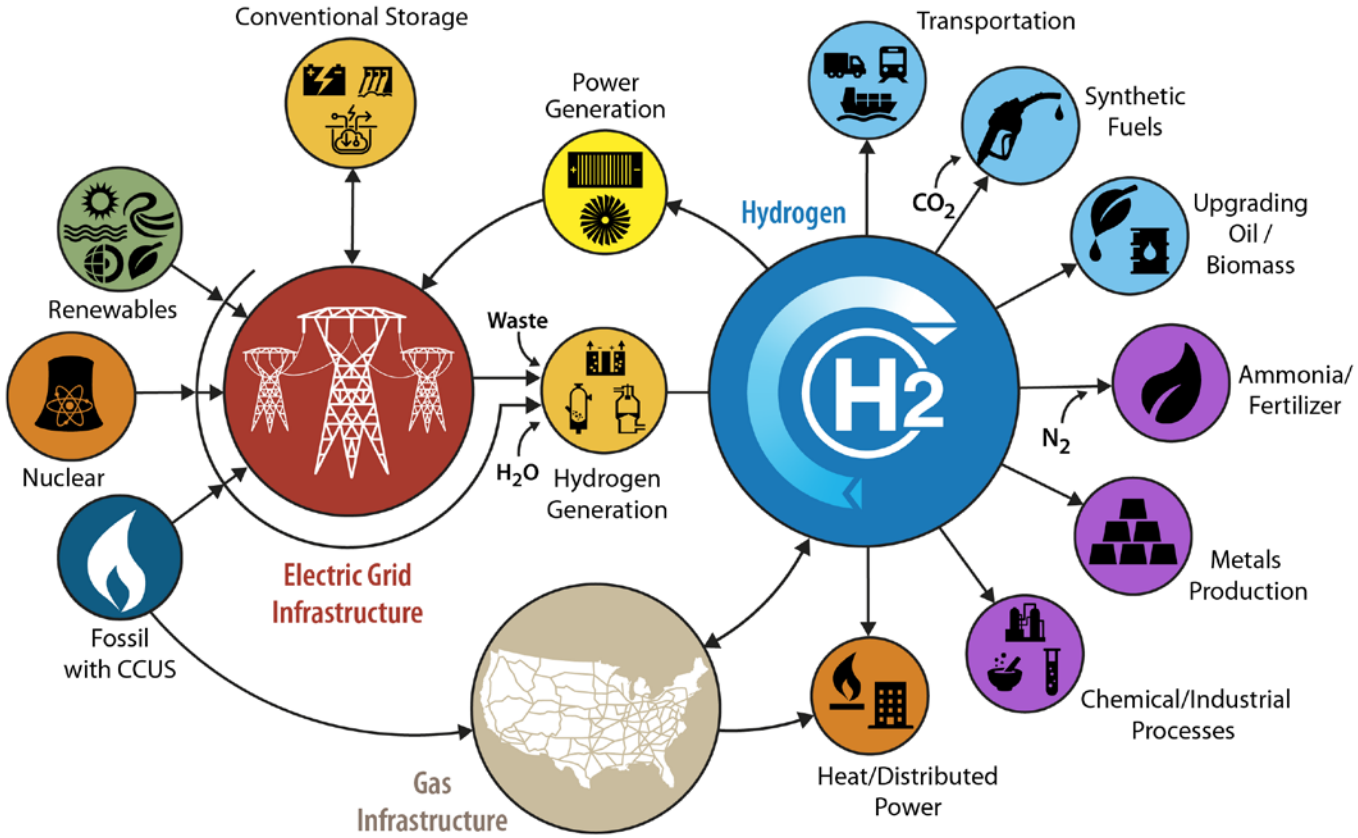
Northwestern University
2014 – 2019

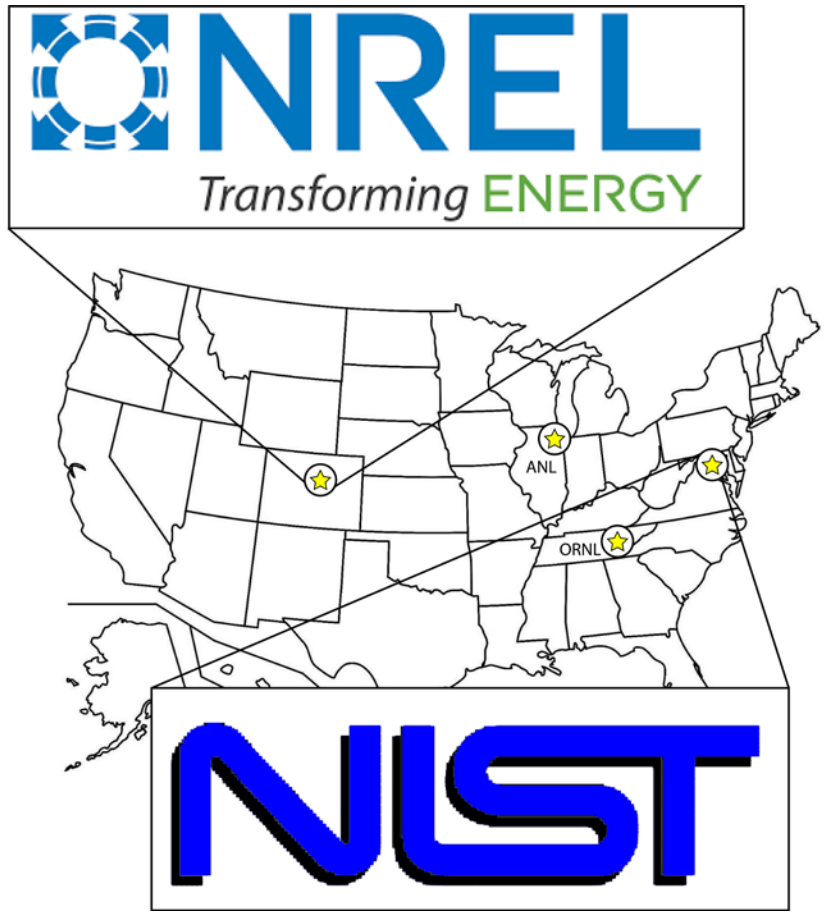
Postdoc Researcher
X-ray and Neutron Scattering

- Dynamic materials for hydrogen storage
- Tuning H_2 enthalpies of adsorption
- Stationary and mobile storage applications

National Renewable Energy Laboratory
Hydrogen Materials Advanced Research Consortium
2019 – present

Developing next generation hydrogen storage materials to help realize the hydrogen energy economy



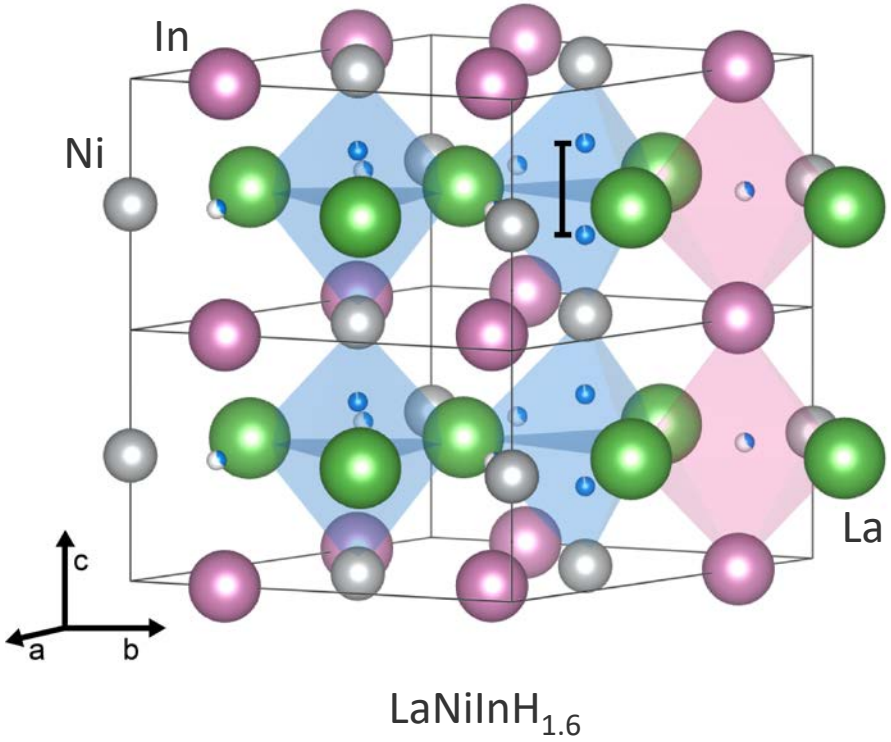


Research Focuses in HyMARC:

- Tuning H_2 enthalpy of adsorption
- Dynamic materials
- Boosting storage capacities

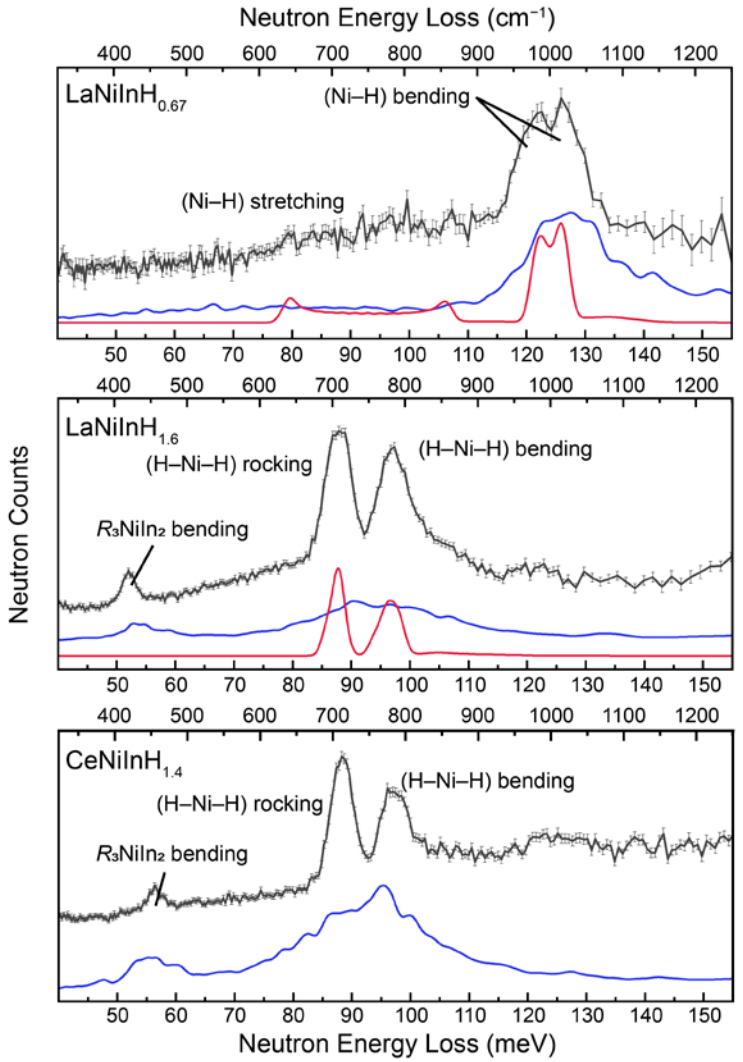
First neutron vibrational spectroscopic investigation of anomalously close H-H contacts in *R*NiInH$_x$

Stationary Storage



$LaNiInH_{1.6}$

V. A. Yartys, V. A. *et al. J. Alloys Compd.* **2002**, *330*, 132–140.
Denys, R. V. *et al. J. Alloys Compd.* **2003**, *356*, 65–68.



Inelastic scattering data
Lattice dynamics simulation
Molecular dynamics simulation

Possible Application: storing excess seasonal/variable renewable energy, large scale backup

Goal: understand how these compounds host anomalously close packed hydride ions

Method: inelastic neutron scattering + first principles calculations-based analysis

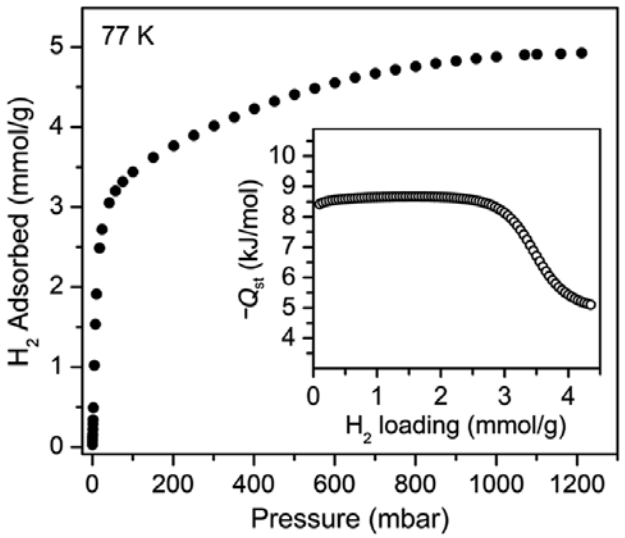
Takeaway: possible route for boosting volumetric capacity determined—screen H^- charges

Klein, R. A.; Balderas-Xicohténcatl, R.; Petter Maehlen, J.; Udovic, T. J.; Brown, C. M.; Delaplane, R.; Cheng, Y.; Denys, R. V.; Ramirez-Cuesta, A. J.; Yartys, V. A. *JALCOM* **2022**, *894*, 162381.

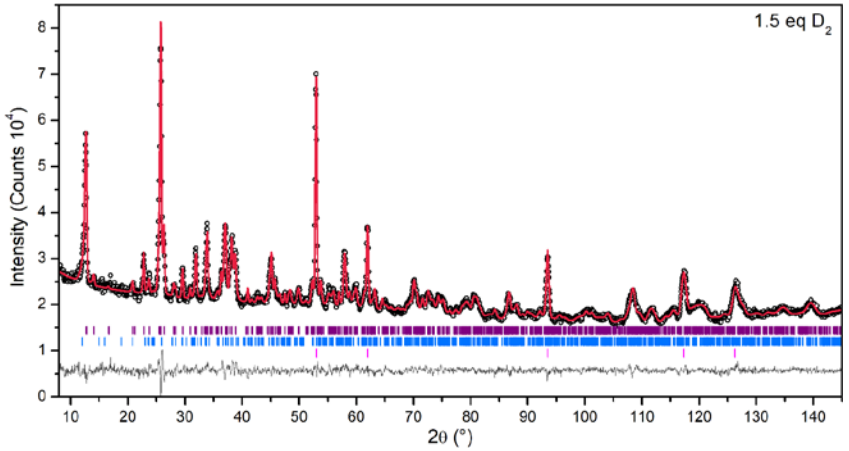
Unconventional tuning of hydrogen enthalpy of adsorption in a metal–organic framework

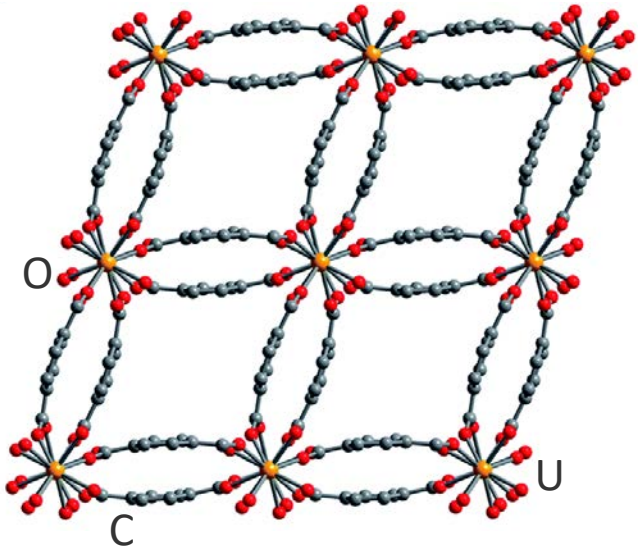
Transportation

H_2 adsorption isotherm data

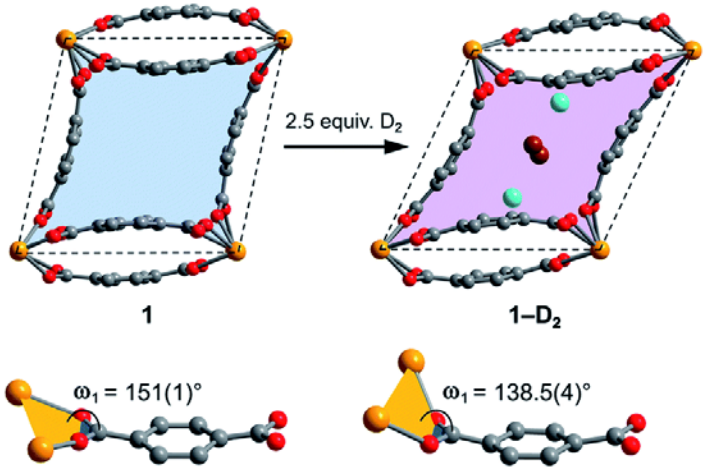


Powder neutron diffraction pattern





U(benzenedicarboxylate)$_2$



Possible Application: heavy duty vehicles, rail

Goal: determine source of high enthalpy of adsorption

Method: powder neutron diffraction-based structure-function analysis

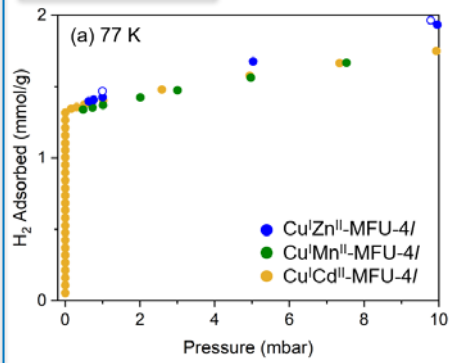
Takeaway: Self-adjusting behavior enhances enthalpy of adsorption

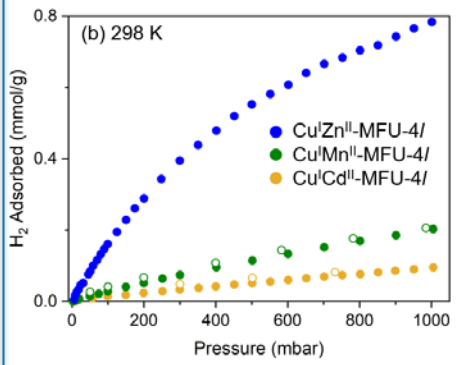
Halter, D. P.; **Klein, R. A.**; Boreen, M. A.; Trump, B. A.; Brown, C. M.; Long, J. R. *Chem. Sci.* **2020**, *11*, 6709–6716.

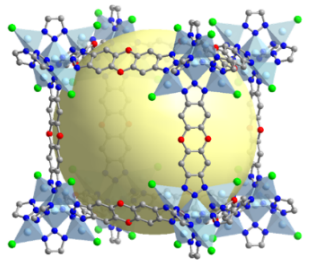
Future direction: tune enthalpy of adsorption in metal–organic frameworks into ideal range for room temperature storage applications

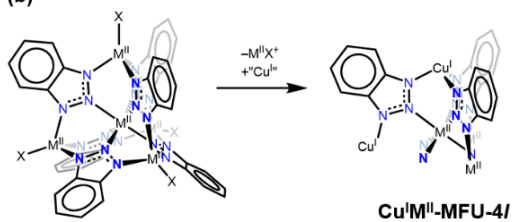
Transportation

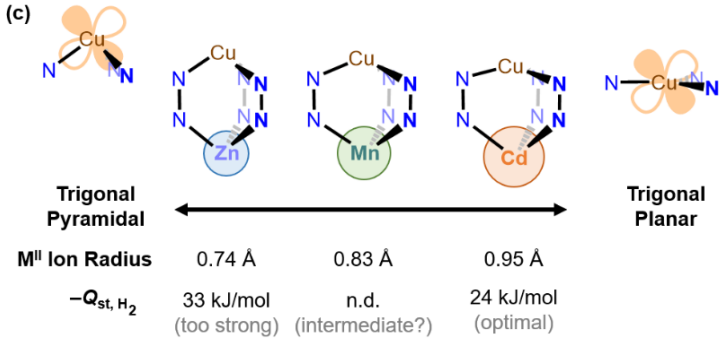
Project 1
M^{II}-MFU-4*l* compounds



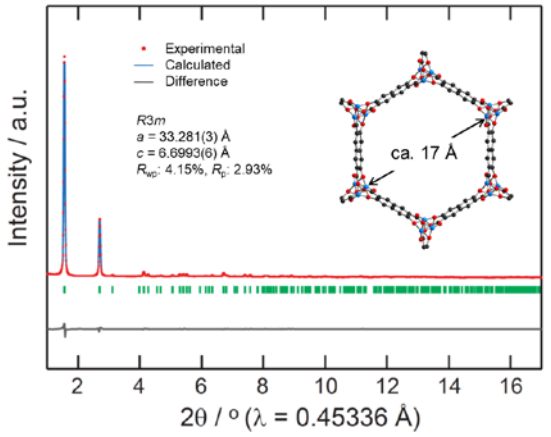


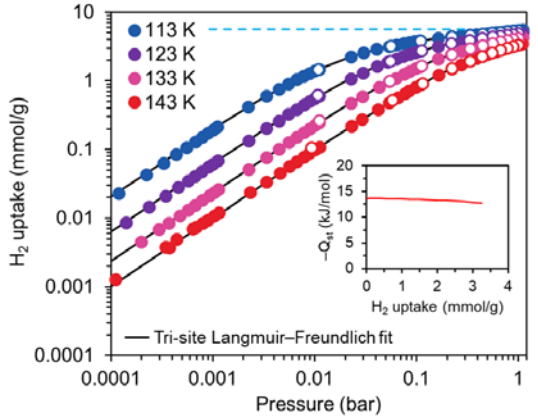




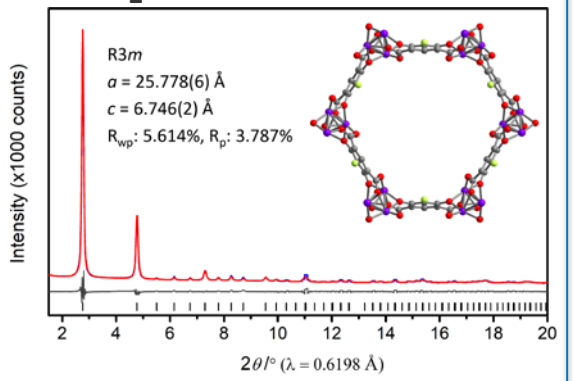


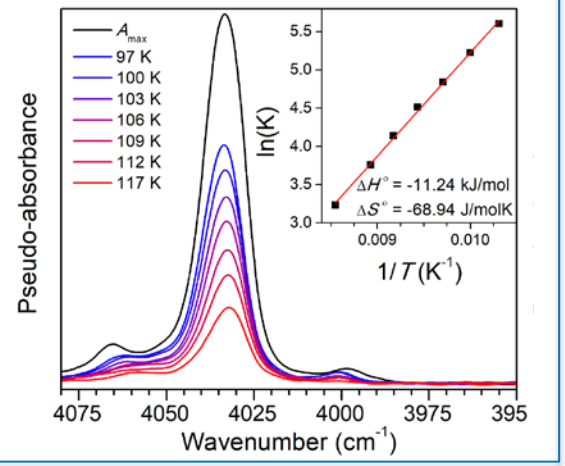
Project 2
M$_2$(dondc) MOFs





Project 3
M$_2$(F-*m*-dobdc) MOFs

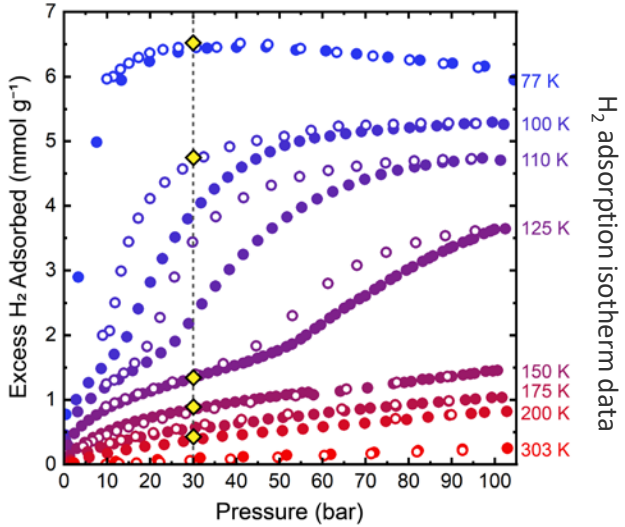




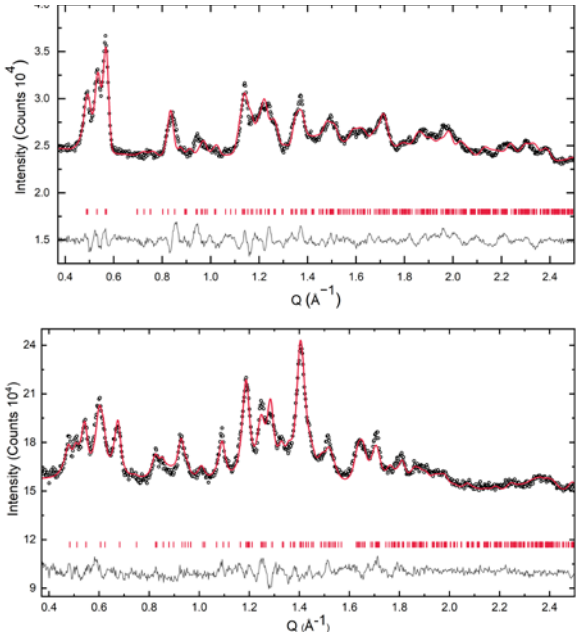
These compounds display nearly ideal enthalpies of adsorption for room temperature hydrogen storage
I will conduct additional measurements at the APS, ORNL, NIST to investigate the storage properties of these materials

Dynamic materials enable access to large useable capacity of stored gas given a small energetic input, provide intrinsic thermal management

Transportation

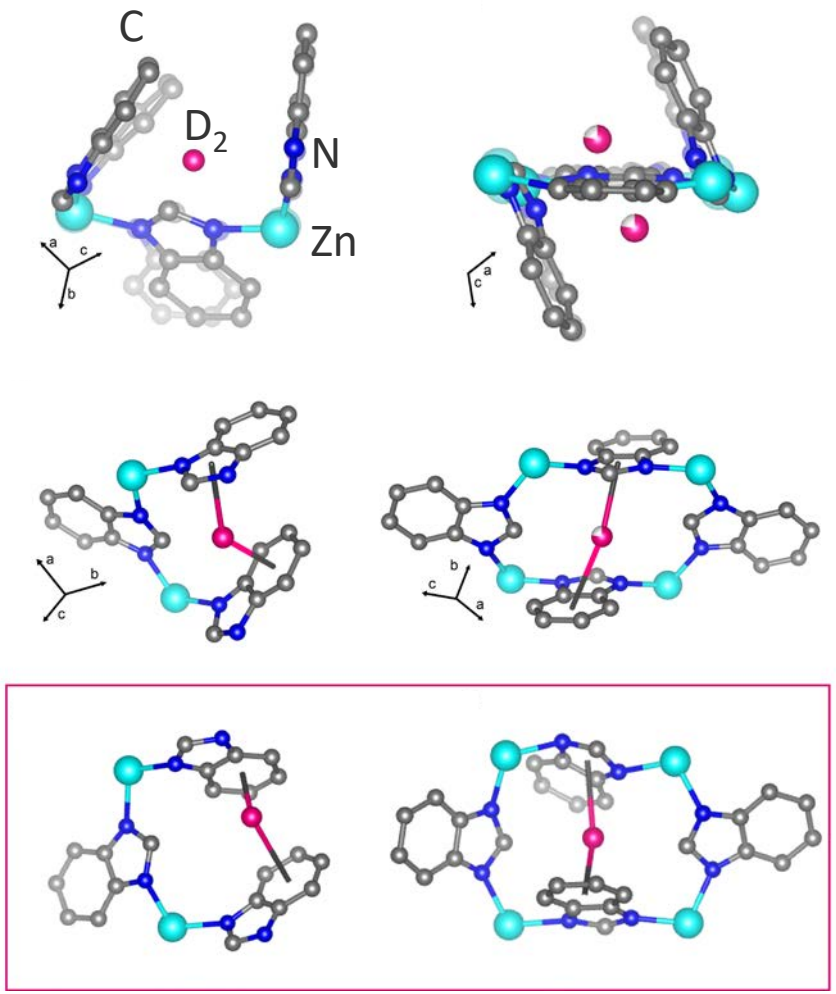


H_2 adsorption isotherm data



Powder neutron diffraction pattens

Zn(benzenedicarboxylate)$_2$ (ZIF-7)



Possible Application: light duty vehicles, marine

Goal: investigate phase transition and find out how to control phase transition conditions

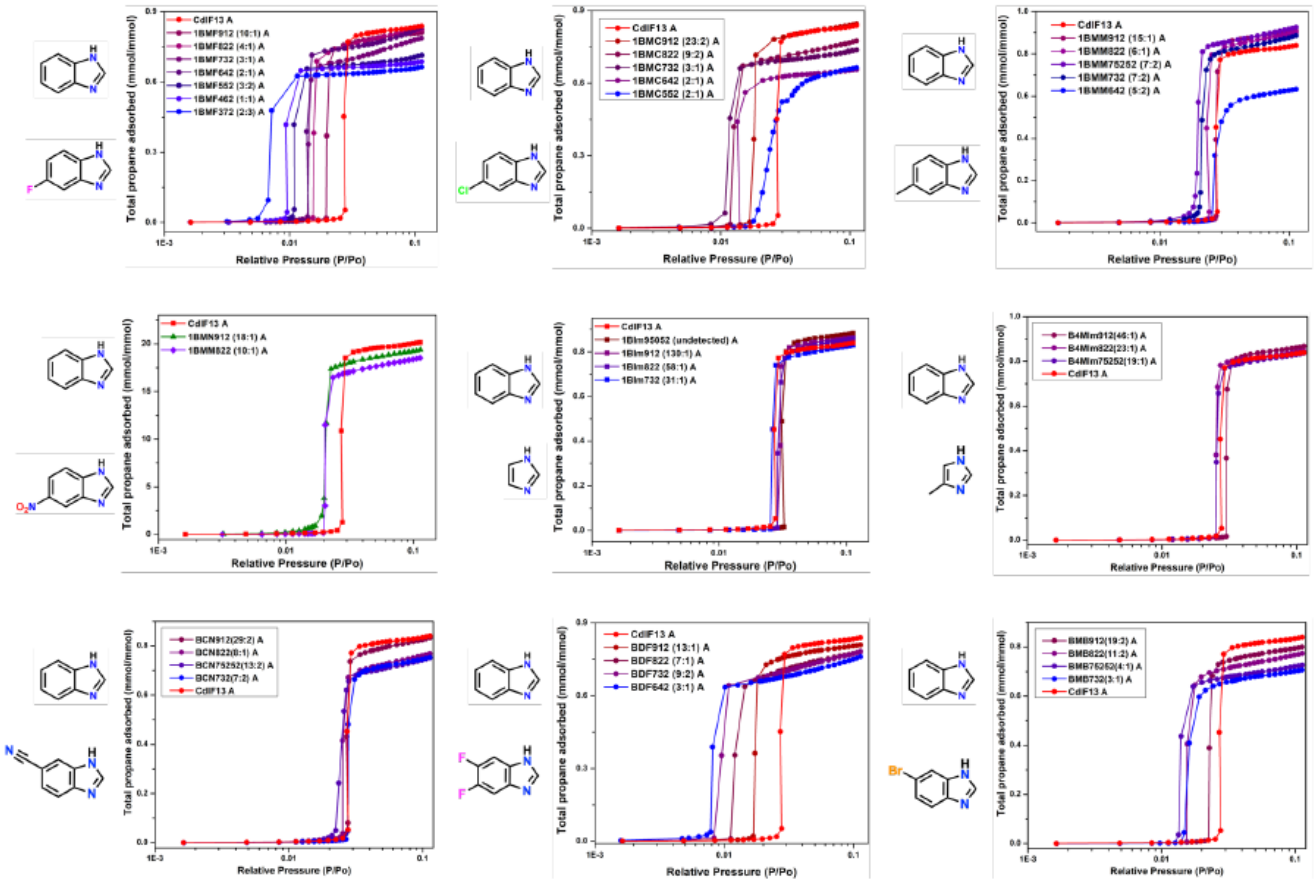
Method: Powder neutron diffraction + isotherm-based structure function analysis

Takeaway: Synthetic route to tuning phase transition conditions determined—functionalize the benzene ring backbone

Klein, R. A.; Shulda, S.; Parilla, P. A.; Morris, W.; Brown, C. M.; Gennett, T.; McGuirk, C. M. *Chem. Sci.* **2021**, *12*, 1562–15631.

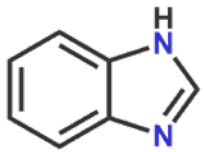
Future direction: Synthetically tune step pressure conditions

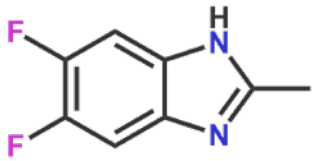
Transportation



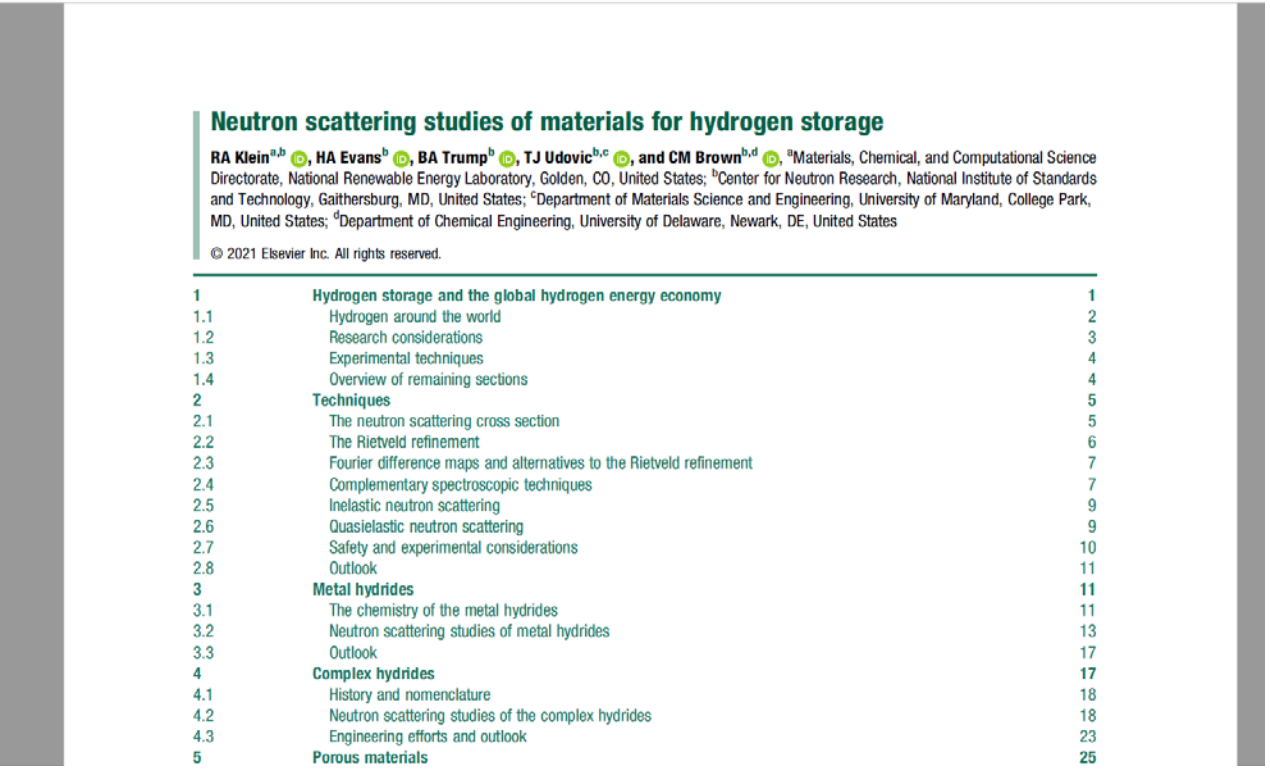
Measurements conducted by Dr. Arijit Halder, Prof. Mike McGuirk for seedling project number DE-EE0008823

As hypothesized, **functionalizing the backbone provides fine synthetic control of phase transition conditions**





Recent Publications



Neutron scattering studies of materials for hydrogen storage

RA Klein[a,b], HA Evans[b], BA Trump[b], TJ Udovic[b,c], and CM Brown[b,d], [a]Materials, Chemical, and Computational Science Directorate, National Renewable Energy Laboratory, Golden, CO, United States; [b]Center for Neutron Research, National Institute of Standards and Technology, Gaithersburg, MD, United States; [c]Department of Materials Science and Engineering, University of Maryland, College Park, MD, United States; [d]Department of Chemical Engineering, University of Delaware, Newark, DE, United States

Klein, R. A.; Evans, H. A.; Trump, B. A.; Udovic, T. J.; Brown, C. M. "Neutron scattering studies of materials for hydrogen storage." *Comprehensive Inorganic Chemistry III, Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, Elsevier, **2021**. https://doi.org/10.1016/B978-0-12-823144-9.00028-5

1. **Klein, R. A.***; Balderas-Xicohténcatl, R.; Maehlen, J. P., Udovic, T. J.; Brown, C. M.; Delaplane, R. G.; Cheng, Y.; Denys, R. V.; Ramirez-Cuesta, A. J.; Yartys, V. A.* *Journal of Alloys and Compounds* **2022**, *894*, 162381. ***Corresponding authors**.
2. **Klein, R. A.***; Carter, C. C.*; Zhou, W.; Udovic, T. J.; Brown, C. M.; Wen, T.-B.; Cundari, T. R.; Yousufuddin, M. *Journal of Alloys and Compounds* **2022**, *894*, 162445.*co-first authors.
3. **Klein, R. A.;** Shulda, S.; Parilla, P. A.; Le Magueres, P.; Richardson, R. K.; Morris, W.; Brown, C. M.; McGuirk, C. M. *Chemical Science*, **2021**, *12*, 15620–15631.
4. **Klein, R. A.;** Evans, H. A.; Trump, B. A.; Udovic, T. J.; Brown, C. M. *Comprehensive Inorganic Chemistry III, Reference Module in Chemistry, Molecular Sciences and Chemical Engineering*, Elsevier, **2021**.
5. Gui, X.; Marshall, M.; Dissanayaka Mudiyanselage, R. S.; **Klein, R. A.;** Chen, Q.; Zhang, Q.; Shelton, W.; Zhou, H.; Brown, C. M.; Cao, H.; Greenblatt, M.; Xie, W. *ACS Applied Electronic Materials* **2021**, *3*, 3501–3508.
6. Episcopo, N.; Chang, P.-H.; Heitmann, T. W.; Wangmo, K.; Fitta, M.; **Klein, R. A.;** Poudel, N.; Gofryk, K.; Zope, R. R.; Brown, C. M.; Nair, H. S. *Journal of Physics: Condensed Matter* **2021**, *33*, 375803.
7. Gui, X.; **Klein, R. A.**; Brown, C. M.; Xie, W. *Inorganic Chemistry* **2021**, *60*, 87–96.
8. Coste, S. C.; Pearson, T. J.; Altman, A. B.; **Klein, R. A.**; Finney, B. A.; Hu, M. Y.; Alp, E. E.; Vlaisavljevich, B.; Freedman, D. E. *Chemical Science* **2020**, *11*, 9971.
9. **Klein, R. A.;** Walsh, J. P. S.; Clarke, S. M.; Liu, Z.; Alp, E. E.; Bi, W.; Meng, Y.; Altman, A. B.; Chow, P.; Xiao, Y.; Norman, M. R.; Rondinelli, J. M.; Jacobsen, S. D.; Puggioni, D.; Freedman, D. E. *Physical Review Letters* **2020**, *125*, 077202.
10. Halter, D. P.; **Klein, R. A.**; Boreen, M. A.; Trump, B. A.; Brown, C. M.; Long, J. R. *Chemical Science* **2020**, *11*, 6709–6716.

Thank you!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Tom Gennett


Wei Zhou


Mike McGuirk


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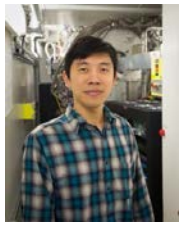
Nick Strange


Timmy Ramirez-Cuesta


Rafael Balderas Xicohténcatl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NREL Transforming ENERGY

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Berkeley UNIVERSITY OF CALIFORNIA

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UT DALLAS The University of Texas at Dallas

NuMat TECHNOLOGIES

National Institute of Standards and Technology
U.S. Department of Commerce

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Thank you!

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