# NANOPOROUS MATERIALS GENOME CENTER PHASE II KICK-OFF MEETING



# UNIVERSITY OF MINNESOTA

#### NANOPOROUS MATERIALS GENOME CENTER PHASE II KICK-OFF MEETING | **PROGRAM**

#### OCTOBER 8 – 9, 2017 | UNIVERSITY OF MINNESOTA

LOCATION:	McNamara Alumni Center, University of Minnesota	
	200 SE Oak St, Minneapolis, MN 55455	
	mac-events.org	

#### Sunday, October 8, 2017

#### Registration opens at 9:30 a.m. in The Commons 10:30 a.m. Meeting begins in the Thomas Swain Room 10:30 a.m. Welcome & update on the Center - Ilja Siepmann 10:45 a.m. Nanoporous Materials Genome: Methods and Software to Optimize Gas Storage, Separation, and Catalysis Laura Gagliardi, Nandini Ananth, Kit Bowen, Aurora E. Clark, Christopher J. Cramer, Michael W. Deem, Omar K. Farha, Jason D. Goodpaster, Maciej Haranczyk, Martin Head-Gordon, Joseph T. Hupp, Jeffrey R. Long, David S. Sholl, Randall Q. Snurr, Donald G. Truhlar, Michael Tsapatsis, and J. Ilja Siepmann 11:15 a.m. Thrust B Top Performing CoRE MOFs with Coordinatively Unsaturated Mg Sites for Selective CO<sub>2</sub>/N<sub>2</sub> Separation Hakan Demir, Emmanuel Haldoupis, Konstantinos D. Vogiatzis, Christopher J. Cramer, J. Ilja Siepmann, and Laura Gagliardi Pore size tuning of poly(styrene-co-vinylbenzyl chloride-co-divinylbenzene) hypercrosslinked Thrust B 11:45 a.m. polymers: insights from molecular simulations Grit Kupgan, Thilanga Liyana-Arachchi, and Coray M. Colina Buffet lunch and discussion of collaborative research projects, The Commons (dining in the 12:15 p.m. Thomas Swain Room) 12:15 p.m. PI Lunch, Gateway Room 1:30 p.m. Control of Electronic Structure and Conductivity in Two-Dimensional Metal-Semiguinoid Thrust C Frameworks of Titanium, Vanadium, and Chromium Michael E. Ziebel, Lucy E. Darago, Jeffrey R. Long 2:00 p.m. Heterogeneous catalysis with metal-organic frameworks: Applications to detoxification of chemical Thrust C warfare agents and hydrogenative reduction of CO<sub>2</sub> Mohammad R. Momeni and Christopher J. Cramer Photocatalytic Capabilities of UiO-66-based Materials 2:30 p.m. Thrust C Xin-Ping Wu, Laura Gagliardi, and Donald G. Truhlar 3:00 p.m. **Coffee Break** 3:30 p.m. Electrocatalytic Coordination Frameworks for Solar Energy Conversion Thrust C Courtney A. Downes and Smaranda C. Marinescu A MOF Identification System for Rapid Search and Informatics Thrust A 4:00 p.m. Benjamin J. Bucior and Randall Q. Snurr Generative models in machine learning and databases Thrust A 4:30 p.m. Alan Aspuru-Guzik 5:00 p.m. **Reception, Heritage Gallery** 6:00 p.m. Buffet dinner, Heritage Gallery Poster session and dessert, The Commons 7:30 p.m. 9:30 p.m. End of poster session

#### NANOPOROUS MATERIALS GENOME CENTER PHASE II KICK-OFF MEETING | **PROGRAM**

OCTOBER 8 – 9, 2017 | UNIVERSITY OF MINNESOTA

# Monday, October 9, 2017

Registration opens at 7:30 a.m. in the Commons Room

7:45 a.m.	Continental breakfast buffet, The Commons (dining in the Thomas Swain Room)		
8:30 a.m.	Meeting begins in the Thomas Swain Room		
8:30 a.m.	Welcome - Ilja Siepmann		
8:40 a.m.	Air Separation with Metalated-Catecholates in Metal-Organic Frameworks Thrust B Samuel Stoneburner, Hakan Demir, Xuan Zhang, Randall Q. Snurr, Omar Farha, Laura Gagliardi		
9:10 a.m.	Projection-based Correlated Wave Function in Density Functional Theory Embedding for Bulk Thrust D Systems		
	<u>Dhabih V. Chulhai</u> and Jason D. Goodpaster		
9:40 a.m.	Factors that influence the electron density of metal atoms deposited on MOFs: short- or long-range Thrust C effects? A computational investigation. Andreas Mavrandonakis and <u>Christopher J. Cramer</u>		
10:10 a.m.	Coffee Break		
10:30 a.m.	<b>Breakout sessions</b> THRUST A: Development of Methods to Accelerate Discovery of Functional Porous Materials <i>Thomas Swain Room</i> Led by: Alan Aspuru-Guzik & Randall Snurr		
	THRUST B: Discovery of Porous Materials for Challenging Chemical Separations <i>Thomas Swain Room</i> Led by: Coray Colina, Ilja Siepmann, & Michael Tsapatsis		
	THRUST C: Discovery of Porous Materials for Challenging Chemical Transformations <i>Gateway Room</i> Led by: Christopher Cramer, Laura Gagliardi, & Joseph Hupp		
	THRUST D: Engineering of Nanoporous Materials with Tailored Electronic Structures <i>Big Ten Room</i> Led by: Jeffrey Long & Donald Truhlar		
11:15 a.m. 12:00 p.m. 12:00 p.m. 2:00 p.m.	Reports from breakout sessions and general discussion, Thomas Swain Room Small working groups Box lunches served, The Commons Adjourn		

Presenters of odd-numbered posters are kindly requested to stay near their posters during the first hour and presenters of even-numbered abstracts are kindly requested to stay near their posters during the second hour of the poster session.

- 1. A MOF Identification System for Rapid Search and Informatics <u>Benjamin J. Bucior</u> and Randall Q. Snurr
- 2. Projection-based Correlated Wave Function in Density Functional Theory Embedding for Bulk Systems <u>Dhabih V. Chulhai</u> and Jason D. Goodpaster
- Top Performing CoRE MOFs with Coordinatively Unsaturated Mg Sites for Selective CO<sub>2</sub>/N<sub>2</sub> Separation <u>Hakan Demir</u>, Emmanuel Haldoupis, Konstantinos D. Vogiatzis, Christopher J. Cramer, J. Ilja Siepmann, and Laura Gagliardi
- 4. Homogeneous and Heterogeneous Cobalt Selenolate Catalysts for the Hydrogen Evolution Reaction <u>Courtney A. Downes</u> and Smaranda C. Marinescu
- Reactive First Principles Monte Carlo Simulations of Nitrogen/Oxygen and Hydrogen Sulfide/Carbon Dioxide Mixtures <u>Evgenii O. Fetisov</u>, Mansi Shah, I-F. Will Kuo, Chris Knight, and J. Ilja Siepmann
- 6. Multirefrence Calculations on Bimetallic Decorated NU-1000 for C-H Activation: Comparison with DFT <u>Carlo Alberto Gaggioli</u> and Laura Gagliardi
- 7. Fast and Accurate Prediction of Hydrogen Adsorption in Nanoporous Materials <u>Arun Gopalan</u>, Benjamin Bucior, Scotty Bobbitt, and Randall Snurr
- 8. Rigorous Projection-based DFT Embedding Methodology <u>Daniel Graham</u>, Dhabih Chulhai, and Jason Goodpaster
- Factors that influence the electron density of metal atoms deposited on MOFs: short- or long-range effects? A computational investigation. Andreas Mavrandonakis and <u>Christopher J. Cramer</u>
- Heterogeneous catalysis with metal-organic frameworks: Applications to detoxification of chemical warfare agents and hydrogenative reduction of CO<sub>2</sub> <u>Mohammad R. Momeni</u> and Christopher J. Cramer

- C2 Adsorption in Zeolites: Sensitivity to Molecular Models
  <u>Mansi S. Shah</u>, Evgenii O. Fetisov, Michael Tsapatsis, and J. Ilja Siepmann
- 12. Air Separation with Metalated-Catecholates in Metal-Organic Frameworks <u>Samuel Stoneburner</u>, Hakan Demir, Xuan Zhang, Randall Q. Snurr, Omar Farha, Laura Gagliardi
- 13. Large-scale screening of MOFs for molecular separations <u>Dai Tang</u>, Ying Wu, Ross J. Verploegh, and David Sholl
- Transport and Adsorption of C8 Aromatics through MFI Nanosheet Membranes <u>Raghuram Thyagarajan</u>, Evgenii O. Fetisov, Robert F. DeJaco, Peng Bai, Michael Tsapatsis, and J. Ilja Siepmann
- Effect of Pore Size, Solvation and Damaging on the Perturbation of Adsorbates: the Mg<sub>2</sub>(dobpdc) Case Study Jenny G. Vitillo and S. Bordiga
- 16. Computational Study of MOF-Supported Metal Catalysts for Ethylene Dimerization <u>Jingyun Ye</u>, Aaron League, Donald G. Truhlar, Christopher J. Cramer, Laura Gagliardi, Varinia Bernales, Omar Farha, Joseph T. Hupp, Zhanyong Li, Aleksei Vjunov, Andrew J. Stevens, Donald Camaioni, John Fulton, Johannes Lercher, Karena Chapman, Ana E. Platero Prats, Leighanne C. Gallington, Mark E. Bowden, and Layla Mehdi
- Control of Electronic Structure and Conductivity in Two-Dimensional Metal-Semiquinoid Frameworks of Titanium, Vanadium, and Chromium <u>Michael E. Ziebel</u>, Lucy E. Darago, Jeffrey R. Long

# ABSTRACTS

LISTED IN ALPHABETICAL ORDER BY FIRST AUTHOR'S LAST NAME

#### Generative models in machine learning and databases

#### Alan Aspuru-Guzik

Department of Chemistry and Chemical Biology, Harvard University

In this presentation, I will discuss my group's current work on machine learning for molecules. In particular, I will discuss issues related to molecular representation, generative models, inverse molecular design, and scalability. I will discuss progress in autoencoders, generative adversarial networks and Gaussian processes. I will discuss my vision for how I hope to help the collaboration in terms of both machine learning and high-performance screening and database tools.

# A MOF Identification System for Rapid Search and Informatics

#### Benjamin J. Bucior and Randall Q. Snurr

Department of Chemical & Biological Engineering, Northwestern University

The Materials Genome Initiative (MGI) envisions faster materials design by combining the strengths of experimental, computational, and database analyses. Developments using the computation-ready, experimental metal-organic framework (CoRE MOF) database show progress toward achieving this goal by enabling high-throughput screening studies to repurpose existing materials for new applications. However, data mining and searches for materials in the database and broader MOF literature can be cumbersome. For example, finding a specific MOF by name requires domain expertise of its multiple synonyms (e.g. Cu-BTC, HKUST-1, and MOF-199 for the same material), which also makes it difficult to integrate multiple sources of data together.

In this talk, we will propose an identification system (dubbed MOFid) derived from a MOF's chemical building blocks and topology. We will introduce the algorithm by example for common MOFs and demonstrate proof-of-concept web interfaces to rapidly search the CoRE MOF database and generate components of the MOFid. We have validated the methodology against hypothetical MOFs of known composition. By facilitating the use of cheminformatics methods, the MOFid has enabled rapid data mining of the CoRE MOF database to extract chemical insights.



# Projection-based Correlated Wave Function in Density Functional Theory Embedding for Bulk Systems

#### Dhabih V. Chulhai<sup>a</sup> and Jason D. Goodpaster<sup>a,b</sup>

<sup>a</sup>Department of Chemistry, University of Minnesota, Twin-Cities <sup>b</sup>Department of Chemical Physics, University of Minnesota, Twin-Cities.

Quantum embedding methods are ideal for describing chemical and biochemical reactions of large systems by using a higher level of theory—such as correlated wave function (WF) method—for the smaller active site, while still accounting for the quantum mechanical interactions with the electrons in the surrounding environment with a more computationally tractable level of theory—such as density functional theory (DFT). We have been developing a projection-based quantum embedding approach that is numerically exact for the embedding of molecular systems. We extend this projection-based technique to systems with periodic boundary conditions, where our results show that we obtain the exact total DFT system energies and densities through embedding. We also describe a finite cluster-in-periodic environment embedding, whereby we may treat the subsystem of interest as an embedded finite molecular subsystem. Such a subsystem may therefore be described using any DFT or WF methods, while still accounting for the periodic environment at a more tractable DFT level of theory. With this method, we can use highly accurate WF methods to describe chemistry localized in small regions in an otherwise bulk material described by DFT.



Figure: An example of cluster CW-in-periodic DFT embedding, where the larger atoms were described using CCSD(T) and the smaller atoms described using DFT with periodic boundary conditions.

# Factors that influence the electron density of metal atoms deposited on MOFs: Short- or long-range effects? A computational investigation.

#### Andreas Mavrandonakis and Christopher J. Cramer

Department of Chemistry, University of Minnesota.

Metal-Organic Frameworks (MOFs) based on  $Zr_6$ -nodes have received considerable interest due to their exceptional thermal, chemical and mechanical stability. Two of the most representative examples are the UiO-66/67 and NU-1000 MOFs, which are constructed from  $Zr_6O_x$  nodes connected via carboxylate ligands. They exhibit coordinated aqua and hydroxyl ligands, which can be used to further deposit well-defined metal sites for catalytic applications.

We are particularly interested in Rh(I) mononuclear sites that can be deposited via reaction of a rhodiumprecursor with a proton from the defect node of the UiO-67 MOF. These Rh(I) sites are catalytically active for ethylene hydrogenation and dimerization reactions. The catalytic activity can be correlated with the electrondonor ability of the support material.

In this work, we will present factors that influence the electron density on the Rh(I) sites, by considering the introduction of several functional groups on the linker and on the node. As descriptor of the electron density on the Rh, we choose to take into account the carbonyl frequencies from the  $-Rh(CO)_2$  moiety, because the Rh-CO frequency is very sensitive to the Rh electron density. Several different functionalities are considered: exchange of the Zr with Hf/Ce, partial dehydration of the node, pre-decoration of the node with Si<sub>x</sub>(OH)<sub>y</sub> and introduction of the -F, -CF<sub>3</sub>, -Cl, -OH and -CN groups in the linker.

Unexpectedly, the computational results reveal that the long-range effects due to the functional groups in the linker have larger magnitude compared to the other short-range effects.

# Top Performing CoRE MOFs with Coordinatively Unsaturated Mg Sites for Selective $CO_2/N_2$ Separation

### <u>Hakan Demir</u>,<sup>a</sup> Emmanuel Haldoupis,<sup>a</sup> Konstantinos D. Vogiatzis,<sup>a</sup> Christopher J. Cramer,<sup>a</sup> J. Ilja Siepmann,<sup>a,b</sup> and Laura Gagliardi<sup>a</sup>

<sup>a</sup> Department of Chemistry, Minnesota Supercomputing Institute, and Chemical Theory Center, University of Minnesota, 207 Pleasant Street Southeast, Minneapolis, MN 55455-0431, United States.

<sup>b</sup> Department of Chemical Engineering and Materials Science, University of Minnesota,421 Washington Avenue SE, Minneapolis, MN 55455-0431, United States.

Metal-organic frameworks (MOFs) are relatively novel, nanocrystalline structures built with the combination of inorganic nodes and organic linkers. Some of their features such as high pore volume, surface area, tunability of inorganic and organic parts, structural flexibility make them very promising for gas storage/separation, catalysis, sensing etc. Among all the MOFs, MOFs with coordinatively unsaturated sites have attracted more attention since specific sorbates can strongly interact with the metal nodes.

To unveil the potential of a subset of MOFs for gas separation, MOFs with open Mg sites in the CoRE (computation-ready experimental) MOF database<sup>1</sup> are screened for selectively capturing  $CO_2$  from a gas mixture of  $CO_2/N_2$  at flue gas conditions. The screening technique relies on building a multi-site Langmuir model for unary adsorption isotherms where the sorbate-sorbent interaction energy near the open Mg site is calculated by periodic density functional theory (DFT) while the rest of the interactions is calculated by TraPPE and UFF forcefields. Afterwards, using ideal adsorbed solution theory (IAST)<sup>2</sup>, the binary adsorption isotherms and selectivities are predicted. Finally, the top performing MOFs are ranked with respect to their  $CO_2/N_2$  selectivities.

#### References

1. Chung, Y. G. et al. Computation-Ready, Experimental Metal–Organic Frameworks: A Tool To Enable High-Throughput Screening of Nanoporous Crystals. Chem. Mater. 26, 6185–6192 (2014).

2. Myers, A. L. & Prausnitz, J. M. Thermodynamics of mixed-gas adsorption. AIChE J. 11, 121–127 (1965).

#### Electrocatalytic Coordination Frameworks for Solar Energy Conversion

#### **<u>Courtney A. Downes</u>** and Smaranda C. Marinescu

Department of Chemistry, University of Southern California, Los Angeles, CA, 90089, USA

Sustainable hydrogen production from water splitting  $(2H_2O \rightarrow 2H_2 + O_2)$  has emerged as a promising pathway for the storage and conversion of renewable energy resources. Solar energy is an attractive alternative to fossil fuels owning to its unparalleled abundance. The ability to store solar energy in H<sub>2</sub>, a clean and carbon-neutral energy carrier, as a method to mitigate its intermittent nature, is vital for the implementation of a sustainable alternative to the fossil-fuel dominated economy. The conversion of water into H<sub>2</sub> requires the design of earthabundant catalysts to replace platinum, which is too scarce and costly for global deployment of solar-to-fuel converting devices. Practical electrochemical and photoelectrochemical energy converting devices also require the immobilization of stable and active hydrogen evolving catalysts onto electrodes and photocathode materials, which remains a significant challenge. Heterogenization of molecular catalysts has emerged as a viable immobilization strategy which combines the advantageous properties of homogeneous and heterogeneous catalysis. We have developed a methodology for the incorporation of metal dithiolate and metal diselenolate molecular catalysts into extended coordination frameworks and have explored their electrochemical H<sub>2</sub> evolving activity in acidic aqueous media. Through simple modifications of the ligand scaffold and/or metal center, we have systematically investigated the ability to tune important catalytic properties of the coordination frameworks such as the overpotential, charge and proton transfer, and efficiency.

# Homogeneous and Heterogeneous Cobalt Selenolate Catalysts for the Hydrogen Evolution Reaction

#### **Courtney A. Downes and Smaranda C. Marinescu**

Department of Chemistry, University of Southern California, Los Angeles, CA, 90089, USA

The ability to efficiently and cost-effectively convert solar energy into molecular hydrogen through water splitting is necessary for meeting rising energy demands and to mitigate the adverse effects of carbon-based fuels on the environment. Earth-abundant homogeneous and heterogeneous electrocatalysts for the hydrogen evolution reaction (HER) have been developed as alternatives to platinum, the state of the art HER catalyst whose high cost and scarcity limit wide-spread use. Hydrogenase enzymes, which catalyze reversible hydrogen production and oxidation in nature near the thermodynamic potential, have served as models for designing biomimetic catalysts for the HER. [NiFeSe] hydrogenases, a subclass of [NiFe] hydrogenase enzymes with a selenocysteine (Sec) replacing a cysteine (Cys) residue terminally bound to the Ni center, display higher activities for the HER and greater O<sub>2</sub>-tolerance than the conventional sulfur only [NiFe] hydrogenases. However, the role selenium plays in these [NiFeSe] hydrogenases is currently unclear. We have recently synthesized a cobalt selenolate coordination polymer based on benzene-1,2,4,5-tetraselenolate (BTSe) that catalyzes the HER in acidic aqueous media. The cobalt selenolate catalyst displayed ~200 mV reduction in the overpotential to reach 10 mA/cm<sup>2</sup> in comparison to the cobalt coordination polymer based on benzene-1,2,4,5tetrathiolate (BTT). Mechanistic studies on the corresponding molecular complex, [Co(bds)<sub>2</sub>][*n*NuB<sub>4</sub>] (where bds = 1,2-benzenediselenolate), have allowed for further understanding into the role of selenium in improving the HER activity.

# First Principles Monte Carlo Simulations for Nanoporous Materials

# Evgenii Fetisov<sup>a</sup>, Mansi Shah<sup>b</sup>, Christopher Knight<sup>c</sup>, and J. Ilja Siepmann<sup>a,b</sup>

<sup>a</sup> Department of Chemistry and Chemical Theory Center, University of Minnesota, Minneapolis, MN <sup>b</sup> Department of Chemical Engineering and Materials Science, University of Minnesota, Minneapolis, MN <sup>c</sup> Leadership Computing Facility, Argonne National Laboratory, Argonne, IL

Predictive modeling of reaction phase and sorption equilibria presents one of the grand challenges in the field of molecular simulation. Difficulties in the study of such systems arise from the need to accurately model both strong, short-ranged interactions leading to the formation of chemical bonds and weak interactions arising from the environment, and to sample the range of time scales involving frequent molecular collisions, slow diffusion, and infrequent reactive events. Here we summarize the efforts of developing simulation methods that combine the advantages of both first principles electronic structure calculations (Kohn–Sham density functional theory) and efficient Monte Carlo phase-space sampling approaches. Using electronic structure methods to calculate the system energy (and, if desired, also the forces) on the fly eliminates the need for empirical potentials and allows for the simulation of systems in novel environments and under extreme conditions. The examples include (i) a novel reactive first principles Monte Carlo (RxFPMC) approach, which is applied to reactive systems under confinement in zeolites and (ii) adsorption simulations of small molecules in metal organic frameworks with open-metal sites.

# Multireference calculations on bimetallic decorated NU-1000 for C–H activation: Comparison with DFT

#### Carlo Alberto Gaggioli and Laura Gagliardi

Department of Chemistry, Chemical Theory Center and Supercomputing Institute, University of Minnesota, 207 Pleasant Street SE, 55455-0431, Minneapolis, Minnesota, USA

In the last years, Zr-based Metal Organic Frameworks (MOFs) have revealed their potential for heterogeneous catalytic applications, due to their high stability.<sup>1</sup> Very recently, the installation of Co(II) ions to the Zr<sub>6</sub> nodes of the MOF NU-1000 has been successfully achieved. This Cobalt decorated NU-1000, upon activation in a flow of O<sub>2</sub> at 230 °C, has been shown to catalyze the oxidative dehydrogenation (ODH) of propane to propene under mild conditions.<sup>2</sup> A DFT study for this Co-NU 1000 catalyzed propane ODH process using a cluster model containing one Co atom has been carried out, elucidating the reaction mechanism.<sup>2</sup> However, polynuclear sites may also be competent for this reaction; in this regard, the mechanism of the ODH with a two Co atoms model has been analyzed, demonstrating the C-H activation of propane to be the rate determining step.<sup>3</sup>

Knowing the mechanism, a further DFT study has been done in order to lower the barrier of the C-H activation step, improving therefore the catalysis.<sup>3</sup> This work has been focused on computing the activation energies by doping one of the two cobalt atoms with another transition metal (namely, Mo, Ti, Mn, Ag, Fe, Ni, Cu, Zn). Encouraging results for Cu and Zn have been found, which lower the activation barrier. After this work, the question of whether DFT could be accurate enough to describe the challenging electronic structure of these systems arose. The quantum chemical study of metals that present electronic states close in energy (which very often happens when dealing with transition metals) requires a detailed analysis in terms of so called multiconfigurational calculations.

In this contribution we focused on the use of multiconfigurational quantum methodologies for analyzing the electronic structure of the cluster model with two cobalt atoms and the models with same valent dopants (Ni, Fe, Cu, Zn), starting from DFT structures. Owing to the large active space required to accurately describe the electronic structure, we used the RAS (restricted active space) approach. For recovering the dynamic correlation, we employed RASPT2 (when affordable) and MCPDFT<sup>3</sup> in top of the RASSCF wavefunction. The activation barriers, spin states energetics as well as descriptors for this catalysis have been analyzed and directly compared with previous DFT studies.

<sup>1</sup>S. Odoh et al., *Chem. Rev.*, **2015**, *115*, 6051- 6111; Y. Huang et al., *Chem. Soc. Rev.*, **2017**, *46*, 126-157; H. Furukawa et al., *Science*, **2013**, *341*, 1230444; D. Yang et al., *J. Am. Chem. Soc.*, **2015**, *137*, 7391-7396; H. G. T. Nguyen et al., *ACS catalysis*, **2014**, *4*, 2496-2500; D. Yang et al., *ACS catalysis*, **2016**, *6*, 235-247; <sup>2</sup>Z. Li et al., *ACS Cent. Sci.*, **2017**, *3*, 31-38; <sup>3</sup>M. Simons et al., in progress; <sup>4</sup>L. Gagliardi et al., *Acc. Chem. Res.*, **2017**, *50*, 66-73.

# Nanoporous Materials Genome: Methods and Software to Optimize Gas Storage, Separation, and Catalysis

#### Laura Gagliardi,<sup>a</sup> Nandini Ananth,<sup>b</sup> Kit Bowen,<sup>c</sup> Aurora E. Clark,<sup>d</sup> Christopher J. Cramer,<sup>a</sup> Michael W. Deem,<sup>e</sup> Omar K. Farha,<sup>f</sup> Jason D. Goodpaster,<sup>a</sup> Maciej Haranczyk,<sup>g</sup> Martin Head-Gordon,<sup>h</sup> Joseph T. Hupp,<sup>f</sup> Jeffrey R. Long,<sup>h</sup> David S. Sholl,<sup>i</sup> Randall Q. Snurr,<sup>f</sup> Donald G. Truhlar,<sup>a</sup> Michael Tsapatsis,<sup>a</sup> and <u>J. Ilja Siepmann</u><sup>a</sup>

<sup>a</sup>University of Minnesota, <sup>b</sup>Cornell University, <sup>c</sup>Johns Hopkins University, <sup>d</sup>Washington State University, <sup>e</sup>Rice University, <sup>f</sup>Northwestern University, <sup>g</sup>Lawrence Berkeley National Laboratory, <sup>h</sup>University of California–Berkeley, <sup>i</sup>Georgia Institute of Technology

The Nanoporous Materials Genome Center (NMGC) discovers and explores microporous and mesoporous materials, including **metal-organic frameworks** (MOFs), **zeolites**, and **porous polymer networks** (PPNs). These materials find use as storage and separation media and catalysts in many energy-relevant processes and their next-generation computational design offers a high-payoff opportunity. Towards that end, the NMGC (i) develops state-of-the-art predictive theories (from high-level electronic structure methods to validated molecular mechanics force fields), hierarchical screening approaches, data-driven discovery tools, applets, databases, and web-based repositories, and (ii) employs them to increase the pace of materials discovery and to understand the fundamentals of interactions and mechanisms that govern performance of nanoporous materials. The goals of the NMGC are advanced by a tight collaboration between leading experimental groups in the synthesis and characterization of nanoporous materials and of computational groups with experience in Monte Carlo and molecular dynamics simulations, electronic structure calculations, data-driven science, scientific computation, and applied mathematics. The majority of the completed and on-going projects benefit from iterative feedback where computational modeling and large-scale data generation/analysis is instrumental for understanding the function of specific nanoporous materials or for discovering materials with optimal properties for subsequent synthesis, characterization, and validation.

The NMGC research efforts have already led to more than 100 publications. In this short presentation, we will highlight key achievements of selected projects leading to the discovery/design of nanoporous materials for separation and catalysis applications and providing improved understanding of the fundamental interactions governing performance of nanoporous materials (see **Figure 1** and **Figure 2**). In addition, we will introduce a first principles Monte Carlo framework that allows for the calculation of adsorption isotherms and reaction equilibria in nanoporous confinements with all interactions described using Kohn-Sham density functional theory. In particular, we will present (i) the adsorption isotherms of  $CO_2$  and  $N_2$  on Mg-MOF-74 where strong interactions of  $CO_2$  with the open-metal site lead to large separation factors and (ii) the chemical equilibria of  $H_2S$  and  $CO_2$  in a sodium-exchanged zeolite where favorable interactions with the cations shift the equilibrium toward the production of  $H_2O$  and OCS.



**Figure 1:** Relationship between optimized deliverable capacity at the 65 bar condition, deliverable capacity at the 35 bar condition, and surface area for MOFs discovered using a genetic algorithm.



**Figure 2:** Electronic structure calculations aid the design of catechol-ligated transition metals as MOF-linkers for gas separations.

In collaboration with the Materials Project, the NMGC has developed the Nanoporous Materials Explorer [https://materialsproject.org/wiki/index.php/Nanoporous Materials Explorer]. This openly accessible web-based tool aids materials discovery and also serves as repository for computational and experimental data generated by the NMGC. NMGC researchers have created a database of computation-ready experimental (CoRE) MOF structures [http://gregchung.github.io/CoRE-MOFs/] and developed a Python tool for the computation of mixture adsorption isotherms using data from isotherms ideal adsorbed unary and the solution theory [https://github.com/CorySimon/pyIAST]. The collaborative NMGC activities have also strengthened the training of a large number of postdoctoral associates and of graduate, undergraduate, and high school students.

Conventional approaches aimed at discovery and development of nanoporous materials for storage, separation, and catalysis applications are hampered by the large number of already synthesized zeolites and MOFs, the much larger number of hypothetical zeolite and MOF structures, and the large number of potential applications, i.e., it would be impossible to synthesize a significant fraction of these materials and to characterize their performance for a variety of applications. The materials genome approach, including genetic algorithms and machine learning tools, developed and employed by the NMGC allows one to explore thousands of materials for a plethora of applications in a relatively short time frame. NMGC research has led to the discovery of zeolites for extraction of ethanol from aqueous solution (Patent Application PCT/US2015/41566), for hydrocarbon dewaxing (Patent Application PCT/US2016/054624), and of MOFs for Kr/Xe and CO<sub>2</sub>/H<sub>2</sub> separation and for ethane-to-ethanol conversion. Over the next year, the NMGC team will continue its collaborative endeavors to discover nanoporous materials with optimal gas storage, separation, and catalytic abilities and to use an integrated computational/experimental approach for unraveling structure/chemistry/function relationships.

#### **Grant Number and Grant Title**

DE-FG02-12ER16362 Nanoporous Materials Genome: Methods and Software

to Optimize Gas Storage, Separation, and Catalysis

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Student(s): Peng Bai, Joshua Borycz, Philip Bunting, Yi Bao, Nicholas Blando, Zachary Brown, Jeff Camp, Yuexing Cui, Lucy Darago, Allison Dzubak, Miguel Gonzalez, Arun Gopalan, Josh Howe, William Isley, Mi Young Jeon, Olga Karagiardi, Marianne Lalonde, Aaron League, Jason Lee, Shaohong Li, Michelle Liu, Sijie Luo, Xi Li, Greg Man, Narbe Mardirossian, Sara Marquez, Dalar Nazarian, Julia Oktawiec, N. Dilip Rangnekar, Doug Reed, Mansi Shah, Meera H. Shete, Huiliang Shi, Cory Simon, Samuel Stoneburner, Jeffrey Sung, Pragya Verma, Bo Wang, Chun-Hung Wang, Jon Witte, Dianne Xiao, Borna Zandkarimi, Hongda Zhang, Tiechen Zhou

Ten Publications Acknowledging this Grant (selected from 105 publications)

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# Multireference calculations on bimetallic decorated NU-1000 for C–H activation: Comparison with DFT

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In the last years, Zr-based Metal Organic Frameworks (MOFs) have revealed their potential for heterogeneous catalytic applications, due to their high stability.<sup>1</sup> Very recently, the installation of Co(II) ions to the Zr<sub>6</sub> nodes of the MOF NU-1000 has been successfully achieved. This Cobalt decorated NU-1000, upon activation in a flow of O<sub>2</sub> at 230 °C, has been shown to catalyze the oxidative dehydrogenation (ODH) of propane to propene under mild conditions.<sup>2</sup> A DFT study for this Co-NU 1000 catalyzed propane ODH process using a cluster model containing one Co atom has been carried out, elucidating the reaction mechanism.<sup>2</sup> However, polynuclear sites may also be competent for this reaction; in this regard, the mechanism of the ODH with a two Co atoms model has been analyzed, demonstrating the C-H activation of propane to be the rate determining step.<sup>3</sup>

Knowing the mechanism, a further DFT study has been done in order to lower the barrier of the C-H activation step, improving therefore the catalysis.<sup>3</sup> This work has been focused on computing the activation energies by doping one of the two cobalt atoms with another transition metal (namely, Mo, Ti, Mn, Ag, Fe, Ni, Cu, Zn). Encouraging results for Cu and Zn have been found, which lower the activation barrier. After this work, the question of whether DFT could be accurate enough to describe the challenging electronic structure of these systems arose. The quantum chemical study of metals that present electronic states close in energy (which very often happens when dealing with transition metals) requires a detailed analysis in terms of so called multiconfigurational calculations.

In this contribution we focused on the use of multiconfigurational quantum methodologies for analyzing the electronic structure of the cluster model with two cobalt atoms and the models with same valent dopants (Ni, Fe, Cu, Zn), starting from DFT structures. Owing to the large active space required to accurately describe the electronic structure, we used the RAS (restricted active space) approach. For recovering the dynamic correlation, we employed RASPT2 (when affordable) and MCPDFT<sup>3</sup> in top of the RASSCF wavefunction. The activation barriers, spin states energetics as well as descriptors for this catalysis have been analyzed and directly compared with previous DFT studies.

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# Fast and Accurate Prediction of Hydrogen Adsorption in Nanoporous Materials

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We present a fast and accurate, semi-analytical method for predicting hydrogen adsorption in nanoporous materials. For any given set of conditions (T, P), the adsorption in a material is calculated as an integral average over all adsorption sites (guest-host interactions) plus the guest-guest contribution as a function of the adsorption pressure (P) and including the effects of confinement. The guest-host interaction energy is calculated using a classical force field [1], where the material is probed using a single-site hydrogen probe [2] to obtain the energy distribution of adsorption sites ( $\rho(E)$ ). Local adsorption at each site is then modeled as a Langmuir isotherm, which when coupled with the density distribution of sites gives an accurate description of adsorption at low loading (Henry's constant). To capture the guest-guest interactions correctly, we consider each adsorbed molecule to have an average coordination number [3], which is taken to be a function of the adsorption conditions (T, P) and the pore size of the material. The coordination number multiplied by the pure component interaction energy of hydrogen accounts for the guest-guest interactions in the local isotherm. The method is tested by predicting hydrogen adsorption on selected metal-organic frameworks (MOFs) from the hypothetical MOF (hMOF) database [4] at 77 K over the broad pressure range of 1 Pa to 100 bar, and the results are compared against predictions from GCMC simulations. Once fully tested, the method can be used to screen large numbers of materials and identify top candidates and design strategies for hydrogen storage and other applications.

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#### Rigorous Projection-based DFT Embedding Methodology

#### Daniel Graham, Dhabih Chulhai, and Jason Goodpaster

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Quantum embedding methods provide a strategy for performing localized high level calculations on chemical subsystems while not incurring the complete computational cost of high level calculations. For many molecular calculations, the region of change is spatially localized to a fragment or subsystem of the larger molecular system. Quantum embedding methods allow high level wave function (WF) calculations on certain subsystems, embedded within the at-large system calculated at a lower level of theory, such as density functional theory (DFT).

I have demonstrated that Huzinaga projection operator based absolute localization WF-in-DFT embedding methods significantly outperform pure DFT methods across a diverse test set and quickly converge to the WF result (attached figure). The absolute localization WF-in-DFT method can be applied to systems at the DFT limit, as long as the size of the WF region is small compared to the system at large.

I plan on several additional studies. I will be studying how subdividing a system differently affects the accuracy and computational cost of the calculation. I am also developing energy gradients to use the WF-in-DFT method for geometry optimization. Additionally, our group is incorporating this method into periodic calculations to provide WF level accuracy in periodic systems with unit cells too large for WF methods; one such example is hydrogen adsorption on metal organic frameworks



#### Pore size tuning of poly(styrene-co-vinylbenzyl chloride-co-divinylbenzene) hypercrosslinked

# polymers: insights from molecular simulations

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Hypercrosslinked polymers (HCPs) are highly porous materials that are attracting increasing interest due to their potential in energy applications. Furthermore, HCPs are considered low-cost and lightweight material with exceptionally high surface area, high thermal stability and relatively robust against chemical degradation. These attractive characteristics from HCPs make them an excellent candidate for important industrial applications such as gas capture, gas storage, catalyst applications, and separation processes.

In this study, the structure-property relationships of HCPs, poly(styrene-co-vinylbenzyl chloride-codivinylbenzene), were investigated using atomistic simulations. A virtual polymerization algorithm, Polymatic, was used to synthesize the HCPs in silico. To ensure the conformity of our simulated samples, the structures were validated with experimental data including BET surface area, micropore volume, and gas loading (H<sub>2</sub> and CO<sub>2</sub>). Furthermore, the influence of the degree of cross-linking on polymer structures was analyzed, and it was observed that, as expected, both the surface area and micropore volume increase as a function of the degree of cross-linking. We also investigated if divinylbenzene molar content in HCPs can be varied to tune the porosity of the polymer structure in order to improve  $H_2/CO_2$  gas separation performance. Specifically, we varied the divinylbenzene content from 0 to 50 mol% and evaluated how structural and gas separation performance changes. Our results demonstrated that divinylbenzene can be used as a porosity tuning agent and it significantly affected the structure and properties of the polymer. However, no significant improvement in  $H_2/CO_2$  gas separation in pressure swing adsorption process with respect to varying divinylbenzene molar content was observed, in contrast with experimental forecast.

Heterogeneous catalysis with metal-organic frameworks: Applications to detoxification of chemical warfare agents and hydrogenative reduction of CO<sub>2</sub>

#### Mohammad R. Momeni and Christopher J. Cramer

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High-area porous metal-organic frameworks (MOFs) with repeating metal oxide nodes, interconnected with organic linkers, are known to be excellent supports and catalysts for a wide variety of applications.<sup>[1]</sup> Recent experimental works<sup>[2]</sup> have shown the extraordinary effectiveness of MOFs in detoxification of phosphorousbased chemical warfare agents (CWAs). However, the most pressing challenge in this field comes from lack of fundamental understanding on catalytic functionality of these materials at both molecular and crystalline levels. In a recent study, a Zr12 dimer MOF has been introduced as a new alternative heterogeneous catalyst to the commonly studied Zr6 secondary building units (SBUs). The reactivity and catalytic activities of these novel super structures, however, need to be explored via careful computational studies. Given the complex nature of the SBU in this MOF, the proton topology and catalytic activity of its Ni<sup>II</sup> and Co<sup>II</sup> hydride deposited catalysts is still unknown. In this work, reactivities of different Zr-MOF SBUs in catalytic hydrolysis of Sarin CWA are thoroughly investigated using both periodic and cluster modeling. Available experimental findings for both hydrated and dehydrated SBUs with different linker designs are fully explained. The results of this comprehensive study enable us to make exciting predictions for achieving more reactive heterogeneous catalysts for hydrolysis of CWAs. Also, catalytic activities of the Ni<sup>II</sup> and Co<sup>II</sup> hydride deposited Zr12 MOFs in hydrogenative reduction of CO<sub>2</sub> to formic acid are thoroughly examined. Our findings in this work are central in appreciating the catalytic roles of MOFs in different applications.

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# C2 Adsorption in Zeolites: Sensitivity to Molecular Models

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Transferable potentials for phase equilibria (TraPPE) form a family of widely used molecular mechanics force fields for a large variety of chemical compounds. We have recently developed an improved united-atom model, called TraPPE–UA2, for ethane and ethylene that accounts for a better distribution of the dispersion interactions in both molecules and the first-order electrostatic interactions in the case of ethylene. Using two sets of models, TraPPE–UA and TraPPE–UA2, the zeolitic structures in the database of the International Zeolite Association are screened for the separation of ethane and ethylene. A detailed analysis, with regards to accessibility of favorable sites and sensitivity to molecular models (also considering TraPPE–EH for ethane), is carried out on the top-performing structures. This study attempts to understand the strengths and shortcomings of the TraPPE force field for predicting mixture adsorption in zeolites.

### Air Separation with Metalated-Catecholates in Metal-Organic Frameworks

# Samuel Stoneburner<sup>a</sup>, Hakan Demir<sup>a</sup>, Xuan Zhang<sup>b</sup>, Randall Q. Snurr<sup>b</sup>, Omar Farha<sup>b</sup>, Laura Gagliardi<sup>a</sup>

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Separation of oxygen and nitrogen in air is of interest in a variety of industrial and environmental applications. Current technology depends on energy-intensive cryogenic separation. Metal-organic frameworks have the potential to enable separations at more accessible temperatures. Metalation of catecholate groups in framework linkers creates low-valency metal centers that can perform novel chemistry. Cluster calculations with DFT and CASPT2 have predicted that most first row transition metals will bind  $O_2$  more strongly than  $N_2$  by over 20 kcal/mol. Trends in the  $O_2$  and  $N_2$  binding are discussed in light of redox interactions between the catecholate, the metal, and the guests. Further screening with second- and third-row transition metals and main group metals is ongoing.



Stoneburner *et al.* Catechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separation. *J. Phys. Chem. C* **2017**, *121* (19), 10463–10469.

### Large-scale screening of MOFs for molecular separations

# Dai Tang<sup>a</sup>, Ying Wu<sup>a,b</sup>, Ross J. Verploegh<sup>a</sup>, and David Sholl<sup>a</sup>

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A series of MOFs from CoRE MOF database with a wide range of pore diameters, metal nodes and topology is investigated with up to 25 molecules of different types. MOFs were screened based on affinity to the adsorbate and selectivity of each molecule pair. Calculation of the Henry's law constant, *K*, by the Widom insertion method quantifies the affinity of each adsorbate in 471 MOFs and identifies high affinity materials. We predicted the adsorption isotherm with a Langmuir isotherm model using the Henry's constant and liquid phase density of adsorbates and compare these predicted isotherms with simulated adsorption isotherms. The selectivity of each molecule pairs was estimated by the ratio of Henry's constant and ranked in descending order. Reasonable measurements exclude the cases with zero accessible void fraction or negative heat of adsorption in both species because they were excluded from the MOF's pores (Fig. 1). By listing the top 20 performing MOFs for each molecule pair, we obtained a number of MOFs predicted to perform molecular separations efficiently for a range of different molecule pairs. One of them, CSD structure code TEDGOA, was found to be the most applicable adsorbent in up to 250 different molecule pairs.



Fig 1. Box and whisker diagrams for the heat of adsorption of each molecule in 471 MOFs.

# Transport and Adsorption of C8 Aromatics through MFI Nanosheet Membranes

# <u>Raghuram Thyagarajan</u><sup>a</sup>, Evgenii O. Fetisov<sup>a</sup>, Robert F. DeJaco<sup>b</sup>, Peng Bai<sup>b</sup>, Michael Tsapatsis<sup>b</sup>, and J. Ilja Siepmann<sup>a, b</sup>

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This work focuses on the separation of mixture of C8 aromatic compounds using MFI-type zeolite membrane. The model membrane system comprises of the 5nm-thick zeolite nanosheet with periodic replications in the *a* and *c* directions. The free surfaces normal to the *b* direction are saturated with silanol groups. We have utilized both first principles and force-field-based molecular dynamics (MD) simulations to understand the diffusion barriers for transport across the zeolite channels. We use an ensemble of framework structures obtained from MD simulations to generate adsorption isotherms for mixtures containing the C8 molecules using Gibbs Ensemble Monte Carlo simulations. We report the adsorption and transport selectivity of p-xylene to other aromatics in the mixture and compare them with experimental observations.

# Effect of Pore Size, Solvation and Damaging on the Perturbation of Adsorbates: the Mg<sub>2</sub>(dobpdc) Case Study

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 $Mg_2(dobpdc)$  (H<sub>4</sub>-dobpdc = 4,4'-dihydroxy-(1,1'-biphenyl)-3,3'-dicarboxylic acid) is an attractive metal organic framework (MOFs), because of its unique performances in carbon dioxide capture and storage if combined with aliphatic amines.<sup>1,2</sup> Its technological relevance is limited by its reputation for fast decomposing in air.<sup>2,3</sup>

In this study the adsorption of CO<sub>2</sub>, CO, and N<sub>2</sub> has been investigated by means of infrared spectroscopy and periodic quantum mechanical B3LYP-D\* calculations.<sup>4</sup> Comparison with literature data on the isomorph MOF-74-Mg, characterized by the shorter dobdc linker, allowed to verify a small, although appreciable effect of the pore size on the perturbation of the adsorbates. Counterintuitively, the energy of interaction increases with the pore size, the origin of this was found in the increase of the dispersion energy component and in the lower framework deformation in Mg<sub>2</sub>(dobpdc).<sup>4</sup> Other aspects that can influence the interaction with guest molecules can be the presence of solvents that can act as competitors with respect to them or structure damaging. For what concerns solvation, the selective poisoning of the main adsorption sites (Mg<sup>2+</sup>) was achieved by preadsorbing CH<sub>3</sub>OH on the open metal sites. Apart two components due to liquid-like CO and direct interaction with Mg<sup>2+</sup> sites respectively, CO adsorption at 100 K was characterized by an IR band due to the interaction of CO with molecules pre-coordinated to Mg<sup>2+</sup>.<sup>4</sup> This band can be used to check the quality of activation procedures for MOFs with open Mg<sup>2+</sup> sites. N<sub>2</sub> and CO adsorption at RT can be on the contrary exploited to check the efficacy of protocols in amine/Mg<sub>2</sub>(dobpdc) composite synthesis. Because of Mg<sub>2</sub>(dobpdc) air-sensitivity, a full IR characterization was also performed after damaging. Surprisingly, although the drastic structural collapse verified by nitrogen volumetry (decrease of 83% in the surface area), the effect of damaging on the infrared spectrum of the MOF was negligible. Similarly, the only change observed in the spectra of the probe molecules was a slightly decrease in their intensity after damaging. This means that IR spectroscopy is not a reliable technique to evidence the degradation of this MOF, at difference of what reported for other systems.<sup>4</sup>



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# Photocatalytic Capabilities of UiO-66-based Materials

#### Xin-Ping Wu, Laura Gagliardi, and Donald G. Truhlar

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Metal-organic frameworks (MOFs) are porous materials with tailorable nodes and organic ligands. MOFs are especially powerful for applications such as catalysis, gas storage, and separation. Most recently, considerable attention has been paid to the electronic nature of MOFs, and the use of MOFs as photocatalysts has raised great interest.

The tunability and porous nature of MOFs appear to be great assets for photocatalytic applications; the former provides greater photoredox possibilities, and the latter facilitates the diffusion of reactants, which then has the potential to overcome the low charge mobility of many nonporous semiconductors. The MOF UiO-66, which demonstrates excellent chemical, mechanical and thermal stabilities, should have superior tunability as it has various potentially functionalizable linkers, and the Zr in the nodes of UiO-66 can be fully or partially substituted by other metals (e.g., Ti, Hf, Th, Ce, and U). Therefore, we considered two possible structural variations of UiO-66 to study the photoredox possibilities.

By performing Kohn-Sham density functional calculations, we obtained two promising results:

- (i) Ce-UiO-66 has a much stronger tendency than other metal-based UiO-66 materials to generate charge-separated states via a ligand-to-metal charge transfer (LMCT). This prolongs the lifetime of the photo-excited state.
- (ii) Functionalizing the linkers in Ce-UiO-66 can tune the photocatalytic capability of this material for different reactions like water splitting and CO<sub>2</sub> reduction without changing its LMCT behavior significantly.

Our findings emphasize the potential usefulness of MOFs in designing photocatalytic devices, and they provide stimulation for the future applications of UiO-66-based photocatalysts.

Computational Study of MOF-Supported Metal Catalysts for Ethylene Dimerization

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Metal-organic frameworks (MOFs) with ultrahigh porosity and large surface area have recently emerged as excellent heterogeneous supports for transition metal catalysts, either through functionalization of the linker or direct modification of the nodes. The mesoporous MOF, NU-1000, is of particular interest due to its chemical and thermal stability as well as its large pore size (~30 Å), which facilitates the diffusion of gaseous molecules. More importantly, the coordinatively unsaturated metal sites at the inorganic nodes provide specific sites for metal oxide species to anchor, enabling the synthesis of a highly dispersed and isolated single-site metal catalysts on the internal surface of NU-1000. Through atomic layer deposition, a highly dispersed Ni catalyst (Ni-NU-1000) was successfully synthesized; it shows good activity and stability for ethylene hydrogenation and was predicted to be a potential catalyst for ethylene oligomerization.[1,2]



In this work, we aim to develop a Ni-NU-1000 catalyst model and from there to identify the catalytic active sites for ethylene dimerization. Furthermore, a variety of metals have been screened to search for potential catalyst candidate the ethylene dimerization with higher selectivity.

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# Control of Electronic Structure and Conductivity in Two-Dimensional Metal-Semiquinoid Frameworks of Titanium, Vanadium, and Chromium

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The design of metal–organic materials displaying permanent porosity in addition to electrical conductivity or magnetic ordering is limited by a lack of systematic studies describing their electronic structure. One strategy for developing new frameworks with long-range electronic interactions is the use of redox-active ligands which form covalent interactions with metal ions. Metal–semiquinoid frameworks containing mixed-valence ligand scaffolds have been established as promising electronic and magnetic materials, but the ability to tune the electronic properties of these frameworks via substitution of the metal ion has not yet been investigated. The synthesis and electronic properties of these materials has been assigned on the basis of spectroscopic, magnetic, and electrochemical characterization, and their charge transport properties are consistent with these electronic properties will be proposed. Overall, these results demonstrate the ability to tune the electronic structure of metal–organic materials and provide insights into the design of new conductive materials.

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			Co-Investigator
	Smaranda Marinescu	University of Southern California	Experimental Integration
			Co-Investigator
	Randall Snurr	Northwestern University	Thrust B Representative*
			Co-Investigator
	INVESTIGATORS		
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_	Omar Farna		
_	Laura Gagilardi		Co-Investigator
_	Magini Harapatuk		Co-Investigator
_		Northwestern University	Co-Investigator
_		University of California, Berkeley	Co-Investigator
	David Sholl	Georgia Institute of Technology	Co-Investigator
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#### NANOPOROUS MATERIALS GENOME CENTER PHASE II KICK-OFF MEETING | ATTENDEE LIST

#### OCTOBER 8 – 9, 2017 | UNIVERSITY OF MINNESOTA

JUNIOR RESEARCHERS, CONTINUED					
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	Bo Yang	University of Minnesota, Gagliardi/Truhlar Group	Postdoctoral Associate		
	Jingyun Ye	University of Minnesota, Truhlar Group	Postdoctoral Associate		

\* Thrust A: Development of Methods to Accelerate Discovery of Functional Porous Materials

Thrust B: Discovery of Porous Materials for Challenging Chemical Separations

Thrust C: Discovery of Porous Materials for Challenging Chemical Transformations

Thrust D: Engineering of Nanoporous Materials with Tailored Electronic Structures

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