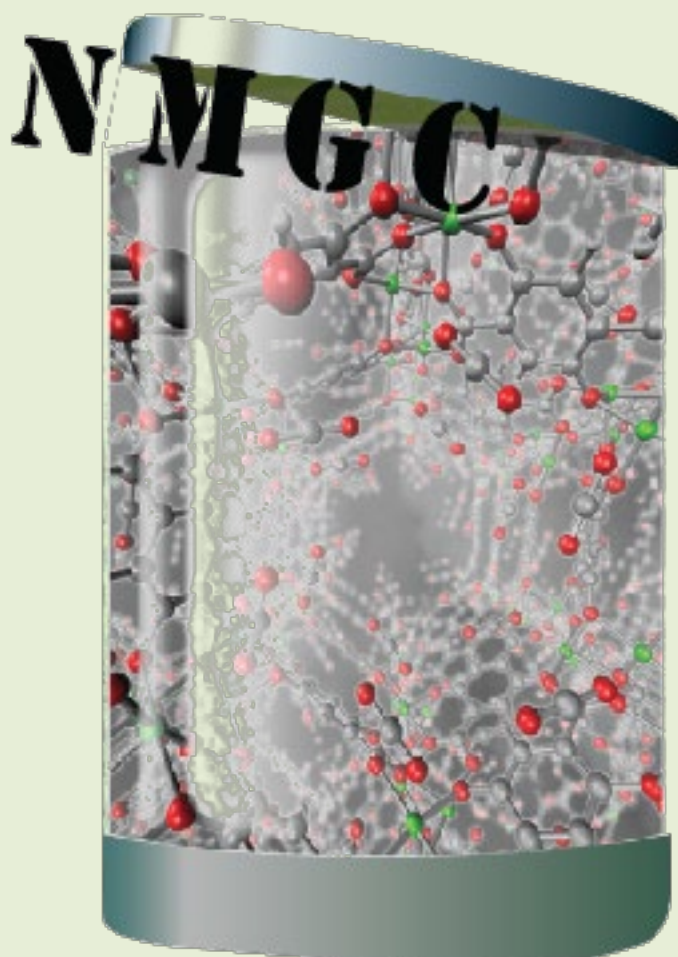


# NANOPOROUS MATERIALS GENOME CENTER

2019 ALL-HANDS MEETING



SEPTEMBER 29 – OCTOBER 1, 2019

UNIVERSITY OF MINNESOTA

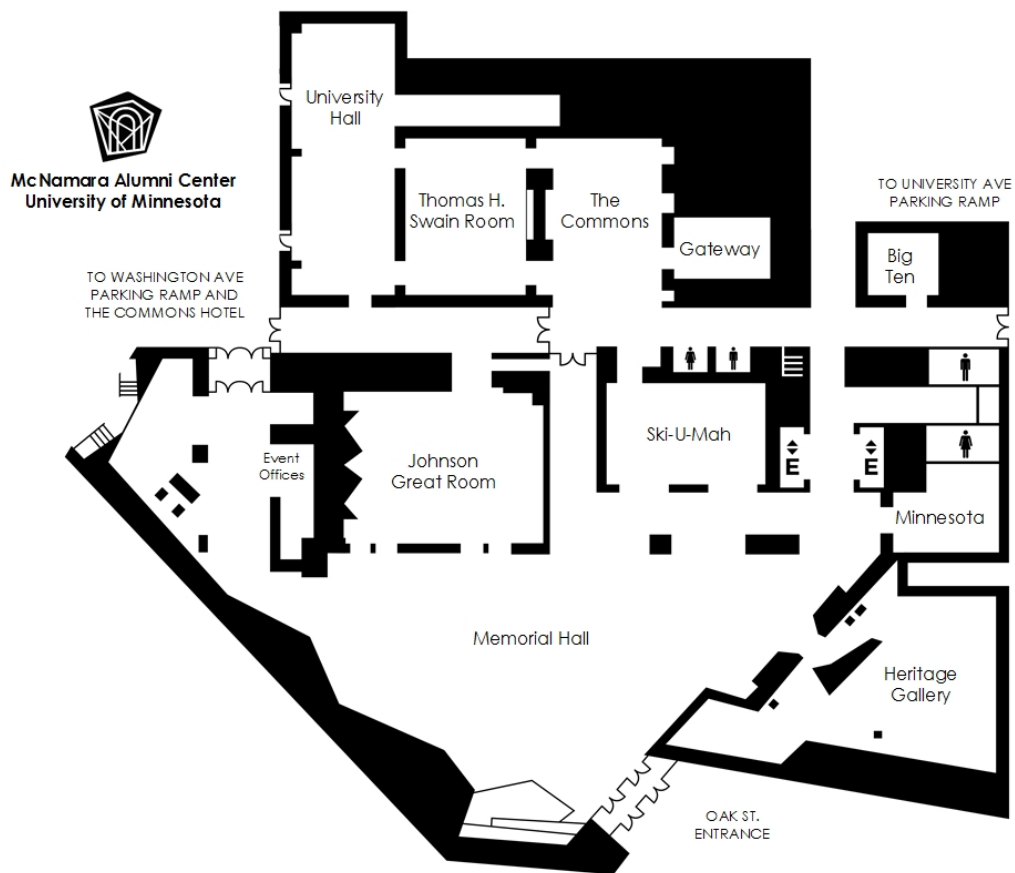
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LOCATION

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

September 29 – October 1, 2019 | University of Minnesota

**Sunday, September 29, 2019**

- 5:30p – 6:30p** Reception (Heritage Gallery)  
**6:30p – 7:30p** Dinner Buffet (Heritage Gallery)  
**7:30p – 9:30p** Poster Session (Commons)

**Monday, September 30, 2019**

*All events held in Thomas Swain Room, unless otherwise noted*

- 8:30a - 9:30a Registration opens, Continental Breakfast available
- 9:30a - 9:50a** **Welcome & Overview**
- 9:50a - 10:20a Maciej Haranczyk  
(A.3) Towards new descriptors, new datasets and synthesizability prediction
- 10:20a - 10:40a Britta Johnson  
(A.2) Quantum Mechanical Studies of Nanoporous Materials
- 10:40a - 11:00a Andrew Sun  
(A.1) Fingerprinting all-silica zeolites for hydrogen storage using meta-learning
- 11:00a - 11:20a WooSeok Jeong  
(A.2) Machine Learning Protocol Development for Automatic Active Space Selection in Multiconfigurational Self-Consistent Field Methods
- 11:20a - 11:40a Michael Ziebel  
(B.1) Energy Storage, Gas Separations, and Charge Transport in Redox-Active Metal–Organic Frameworks
- 11:45a - 1:00p** **Buffet Lunch**
- 11:45a - 1:00p PI Lunch (Ski-U-Mah)
- 1:00p - 1:15p Scientific Advisory Board Meeting, with Director Siepmann (Ski-U-Mah)
- 1:15p - 1:45p Executive Committee Meeting (Ski-U-Mah)
- 1:00p - 2:00p** **Small working groups**
- 2:00p - 2:20p Riki Drout  
(B.1) Isothermal Titration Calorimetry and Zirconium-based Metal–Organic Frameworks: A Thermodynamic Investigation of Uremic Toxin Adsorption
- 2:20p – 2:40p Roshan Ashokbhai Patel  
(C.1) Theoretical Insights into Solvent Effects on Sugar Transformation Chemistry in Modified UiO-66
- 2:40p – 3:00p Keying Chen  
(C.2) Hydrogen Evolving Activity of Dithiolene-Based Metal-Organic Frameworks
- 3:00p – 3:20p Break
- 3:20p – 3:40p Carlo Alberto Gaggioli  
(D.1) Computational Study of the Electronic Structure and Conductivity in 2D Metal-Semiquinoid Frameworks of Fe, Ti, V and Cr
- 3:40p – 4:00p Riddhish Pandharkar  
(D.2) Spin-State Ordering in Metal-Based Compounds Using the Localized Active Space Self-Consistent Field Method
- 4:00p – 4:20p Tyler R. Josephson  
(B.1) Molecular Simulations and Machine Learning for Multicomponent Adsorption: BTEX Separation with Zeolite Membranes
- 4:20p - 5:00p** **Small working groups**
- 6:00p - 9:00p** **Dinner, Lake Monster Brewing, Emconada Food Truck** (550 Vandalia St #160, Saint Paul, MN 55114)  
Light Rail Directions: Take the Green Line from East Bank Station to Raymond Ave Station, then walk 0.6 miles (head SE on University Ave, right on Vandalia St, left on Wabash Ave)

**Tuesday, October 1, 2019**

- 8:00a - 1:00p Small working groups; Meeting space available in Smith Hall rooms 117/119 and 101J

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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. Dylan M. Anstine**  
Screening PIM-1 Performance as a Membrane For Binary Mixture Separation of Gaseous Organic Compounds
- 2. Brianna A. Collins**  
Modeling Magnetic Metal Organic Frameworks Using Density Functional Theory
- 3. Jiaxin (Dawn) Duan**  
Engendering and Engineering Electrical Conductivity in Metal-Organic Frameworks
- 4. Arun Gopalan**  
Fast and Accurate Prediction of Hydrogen Adsorption in Nanoporous Materials
- 5. Daniel Graham**  
Huzinaga WF-in-DFT Embedding for MOFs
- 6. Andrew Johannesen**  
Generation of Machine Learning Potentials for Small Molecule Homogeneous Systems Using Neural Networks
- 7. Tyler R. Josephson**  
Molecular Simulations and Machine Learning for Multicomponent Adsorption: BTEX Separation with Zeolite Membranes
- 8. Srinivasu Kancharlapallia**  
High-Quality Partial Atomic Charges for MOFs from Machine Learning
- 9. Sai Govind Hari Kumar**, *presenting on behalf of Zhenpeng Yao*  
Automated Metal-Organic Framework Discovery Platform for Clean Energy Applications  
& A 3D Convolutional Neural Network based Variational Autoencoder for Gas Storage Prediction of Zeolites
- 10. Zhao Li**  
Machine Learning Using the Guest/Host Energy Histogram to Predict Alkane Adsorption and Xenon/Krypton Separation
- 11. Hung Q. Pham**  
Electronic Structure of Solid-State Materials with Density Matrix Embedding Theory
- 12. Saied Md Pratik**  
Metal-Organic Frameworks for Photocatalytic and Optoelectronic Applications
- 13. Ravithree D. Senanayake**  
Gold Nanoparticles in the NU-1000 Metal Organic Framework: Structures and O<sub>2</sub> Activation
- 14. Dai Tang**  
Prediction Model for Adsorption in Metal-Organic Frameworks Developed by Machine Learning Algorithm: Separation of Near-Azeotropic Species
- 15. Michael Ziebel**  
Energy Storage, Gas Separations, and Charge Transport in Redox-Active Metal–Organic Frameworks

# ABSTRACTS

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LISTED IN ALPHABETICAL ORDER BY FIRST AUTHOR'S LAST NAME

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## **Screening PIM-1 performance as a membrane for binary mixture separation of gaseous organic compounds**

Dylan M. Anstine<sup>a,b</sup>, Alexander G. Demidov<sup>b,c</sup>, Nicholas F. Mendez<sup>b,d</sup>,  
Wesley J. Morgan<sup>b,d</sup>, and Coray M. Colina<sup>a,b,c</sup>

<sup>a</sup> Department of Materials Science and Engineering, University of Florida

<sup>b</sup> George and Josephine Butler Polymer Research Laboratory, University of Florida

<sup>c</sup> Department of Chemistry, University of Florida

<sup>d</sup> Department of Chemical Engineering, University of Florida

Developing microporous polymeric membranes for the separation of a diverse set of organic species can have a profound impact on many industrial fields. This study reports data for unary/binary adsorption and membrane separation performance for acetaldehyde, acetone, methane, methanethiol, propane, and propene studied with a polymer of intrinsic microporosity (PIM-1). The data is reported at 300 K for the pure gases, 15 unique binary pairs, and at 3 molar ratios (45 in all), which required a total of 2573 independent simulations. Based on the potential complexities associated with binary adsorption processes, we describe a statistical approach that can be broadly applicable in identifying system equilibration and overall contribute to predictions with increased fidelity, enabling high-throughput screening. The adsorption selectivity for all binary pairs studied was found to be correlated with the competing polarity of the molecules composing the binary mixture. In addition, we report several PIM-1 binary mixture membrane performance metrics, such as permselectivity, for the hydrocarbon gases evaluated. Considering the range of available experimental data, the membrane performance metrics reported are in good agreement and highlight the ability of molecular simulation screening studies to aid in the design of polymeric membranes for separations of binary mixtures composed of diverse chemical species.

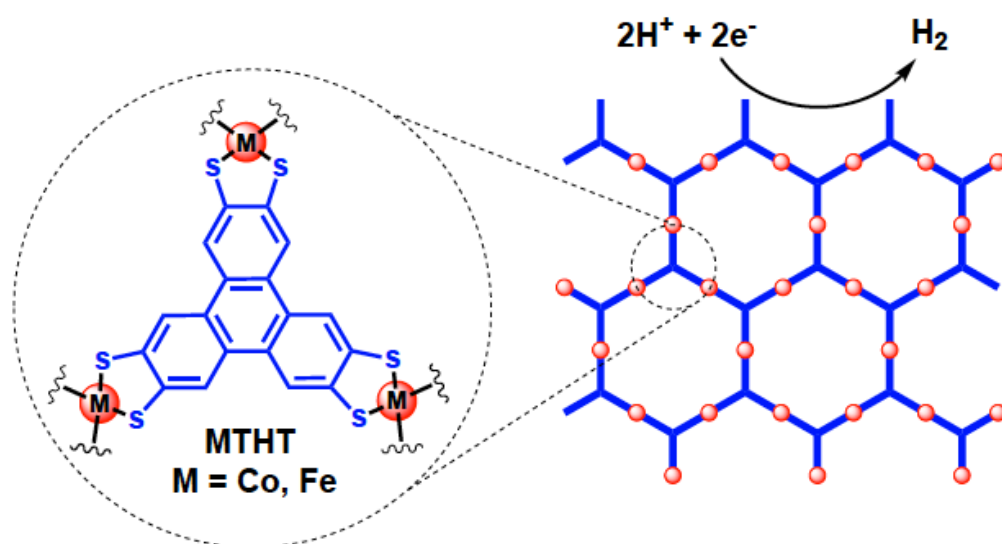
## Hydrogen Evolving Activity of Dithiolene-Based Metal-Organic Frameworks

Keying Chen<sup>a</sup>, Courtney A. Downes<sup>a</sup>, Jason D. Goodpaster<sup>b</sup>, and Smaranda C. Marinescu<sup>a</sup>

<sup>a</sup> Department of Chemistry, University of Southern California

<sup>b</sup> Department of Chemistry, University of Minnesota- Twin Cities

Electrocatalytic systems based on metal-organic frameworks (MOFs) have attracted great attention due to their potential application in commercially viable renewable energy-converting devices. Two-dimensional dithiolene-based MOFs are among the most active MOFs for the electrocatalytic hydrogen evolution reaction (HER). We have recently shown that cobalt 2,3,6,7,10,11-triphenylenehexathiolate (**CoTHT**) framework is an efficient HER catalyst in pH 1.3 aqueous media. In addition to the experimental studies, density functional theory (DFT) calculations were also applied to understand the mechanism of the HER for **CoTHT**. In view of the excellent HER activity of **CoTHT**, we subsequently investigated a series of analogous MOFs where the metal centers are replaced by iron or a mixture of cobalt and iron. The incorporation of both metal centers is verified by various spectroscopic techniques, and the integrity of the crystalline structure is maintained regardless of the metal compositions. However, unlike **CoTHT**, the **FeTHT** framework exhibits minimal activity towards the HER. In addition, the performance of the mixed-metal MOFs is adversely influenced by the incorporation of Fe, where materials with higher Fe content display lower activity and diminished long-term stability. The poor activity of **FeTHT** and the detrimental role of the **FeTHT** domains within the mixed-metal frameworks are speculated to be a result of a conductivity-switching process, which has not been observed for analogous electrocatalytic systems. These results suggest that great caution should be taken when designing MOF-based electrocatalysts, as bulk properties such as conductivity might be altered under electrocatalytic operating conditions thus influencing their overall catalytic performance.



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## **Modeling Magnetic Metal Organic Frameworks using Density Functional Theory**

Brianna A. Collins and Jason D. Goodpaster

Department of Chemistry, University of Minnesota-Twin Cities

We use spin-polarized Density Functional Theory (DFT) to study the electronic structure and magnetic properties of Metal-Organic Frameworks (MOFs). MOFs are porous nanomaterials that contain metal nodes that are attached to organic linkers. As a result of their construction, MOFs offer intrinsic porosity and tunability of their chemical and electronic structure that is not present in traditional magnetic materials. We aim to understand, characterize, and utilize MOFs as magnetic materials. DFT is an attractive method to study magnetic materials because the spin density, that gives rise to magnetic moments, is well defined. Additionally, DFT is computationally efficient and can be applied to these large MOF systems. However, there are well-known obstacles with modeling magnetic moments in DFT, such as the lack of proper electron localization. Therefore, we apply various DFT methods to build an appropriate protocol for the study of magnetic MOFs.

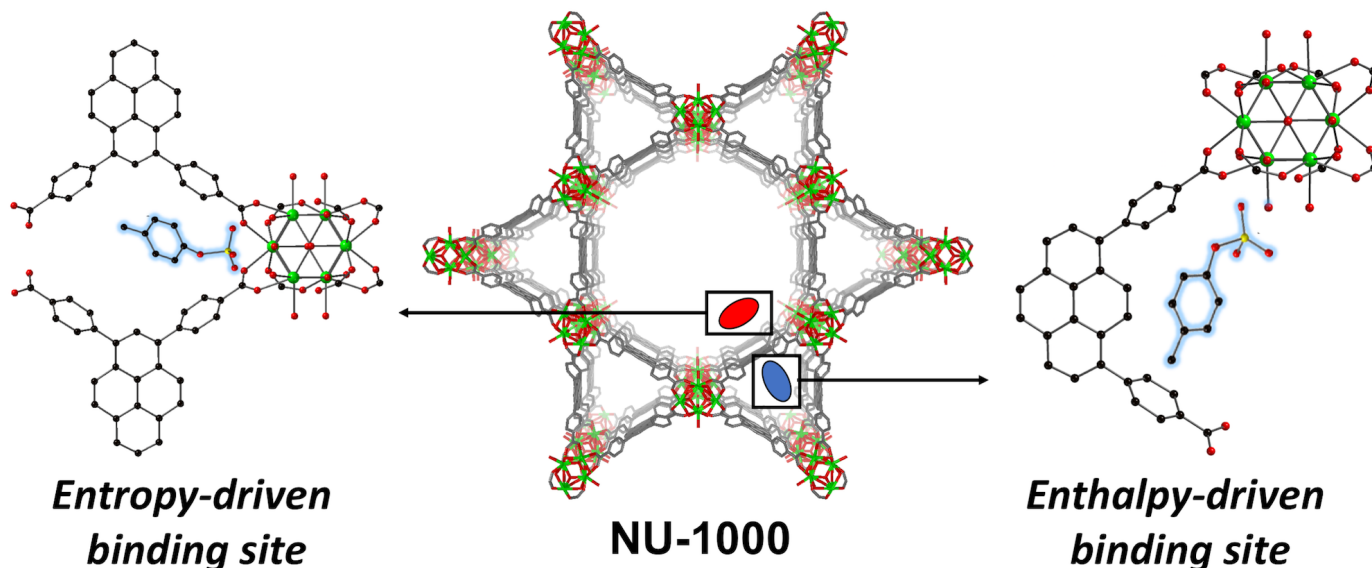


## Isothermal Titration Calorimetry and Zirconium-based Metal–Organic Frameworks: A Thermodynamic Investigation of Uremic Toxin Adsorption

Satoshi Kato, Riki J. Drout, and Omar K. Farha

Department of Chemistry and International Institute of Nanotechnology, Northwestern University

Recent efforts have examined metal–organic frameworks (MOFs) as sorbents for removing pollutants or trace chemicals like pharmaceuticals from aqueous media. However, few studies have systematically investigated the energetics of interactions between chemical toxins and MOF-based sorbents. To this end, we quantified the thermodynamic parameters associated with the adsorption of uremic toxins, namely *p*-cresyl sulfate and indoxyl sulfate, onto zirconium-based MOFs using isothermal titration calorimetry (ITC). A MOF comprising a pyrene-based linker, NU-1000, possesses two distinct adsorption sites which display different binding affinities, one in which the enthalpy term dominates and the other in which the entropy term dominates. ITC measurements revealed that a concerted interaction which embodies both favorable enthalpic and entropic contributions is critical for designing a high capacity MOF adsorbent.



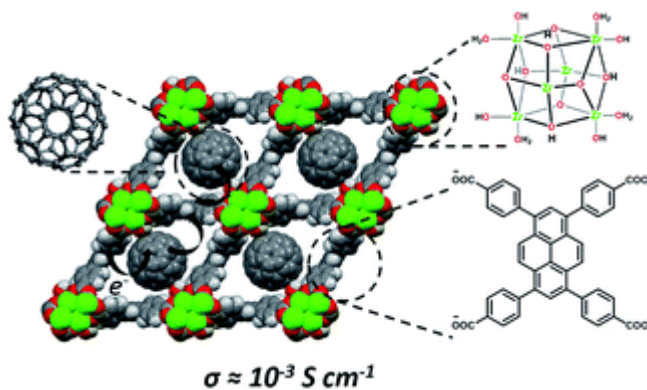
## Engendering and Engineering Electrical Conductivity in Metal-Organic Frameworks

Jiixin (Dawn) Duan<sup>a</sup>, Subhadip Goswami<sup>a</sup>, Chung-Wei Kung<sup>b</sup>, and Joseph T. Hupp<sup>a</sup>

<sup>a</sup> Department of Chemistry, Northwestern University

<sup>b</sup> Department of Chemical Engineering, National Cheng Kung University

Intrinsically insulating Metal-Organic Frameworks (MOFs) can be rendered electrically conductive (i.e., made functionally semiconducting). Electronic conductivity, especially when achieved with retention of MOF porosity, could make MOFs effective for applications in electrocatalysis, light-to-electrical energy conversion, chemical sensing, and/or nanoscale chemo-responsive electrical switching, as well as facilitate functional integration of MOFs within specialized microelectronic devices. Notably, the magnitude of MOF electronic conductivity can be engineered. To engender electronic conductivity, we have exploited solution-assisted incorporation of suitable guest molecules into various MOFs. The post-synthetic guest incorporation methods maintained the crystallinity of the MOFs while introducing donor/acceptor charge-transfer interactions. By changing the electron donors and acceptors, we can tune the charge-transfer band gap and thus engineer the electronic conductivity. In principle, careful attention to MOF topology and to siting of molecular guests (electron donors or acceptors) could also lead to control over conduction dimensionality, e.g. 1D vs. 2D vs. 3D vs. fractal conduction, as well as control over the magnitude of any spatial anisotropy associated with less than uniform, 3D conduction. It is conceivable that insights garnered from studies of electronic conductivity can inform the design of porous MOFs displaying useful thermal conductivity. Computational studies have been initiated by Debmalya Ray and other members of the Gagliardi and Cramer research groups at the University of Minnesota.



## Computational Study of the Electronic Structure and Conductivity in 2D Metal-Semiquinoid Frameworks of Fe, Ti, V and Cr

Carlo Alberto Gaggioli and Laura Gagliardi

Department of Chemistry, Chemical Theory Center and Supercomputing Institute, University of Minnesota-Twin Cities

In the past years, an increasing number of Metal–Organic Frameworks (MOF) has been shown to display electronic conductivity that can be exploited for several applications, such as battery electrodes, thermo-electrics, electrochemical sensors, electrocatalysts.<sup>[1]</sup> There have been proposed several ways to achieve electronic conductivity in MOFs, such as using metal thiolate chains, infinite  $\pi$ – $\pi$  stacking, donor–acceptor charge transfer chains, and  $\pi$ – $d$  conjugated square planar metal sites. Another strategy that led to improved conductivities consists of using mixed-valence units that repeat in one, two, or three-dimensions. MOFs are particularly appealing cause it is possible to tune their surface chemistry and electronic structure via modification of metal, ligand, and network topology.

Recently, it has been shown that mixed valence 2D-Metal Semiquinoid Frameworks are an appealing class of materials for conductivity applications, and the Fe, Ti, V and Cr phases have been analyzed experimentally, revealing an exciting high tunability of the electronic structure and conductivity.<sup>[2]</sup> In this contribution, we employ computational methods to understand the electronic structure and the mechanism of conductivity in these materials. A systematic DFT study have been performed in order to find a reliable computational strategy that can reproduce experimental data, in order to be predictive for the analysis of new materials not yet synthesized.

### References

[1] (a) Sun, L.; Campbell, M. G.; Dinca, M. *Angew. Chem. Int. Ed.* **2016**, *55*, 3566. (b) D’Alessandro, D. M.; Kanga, J.; Caddy, J. S. *Aust. J. Chem.* **2013**, *64*, 718. (c) Morozan, A.; Jaouen, F. *Energy Environ.Sci.* **2012**, *5*, 9269. (d) Erickson, K. J.; Léonard, F.; Stavila, V.; Foster, M. E.; Spataru, C. D.; Jones, R. E.; Foley, B. M.; Hopkins, P. E.; Allendorf, M. D.; Talin, A. A. *Adv. Mater.* **2015**, *27*, 3453.

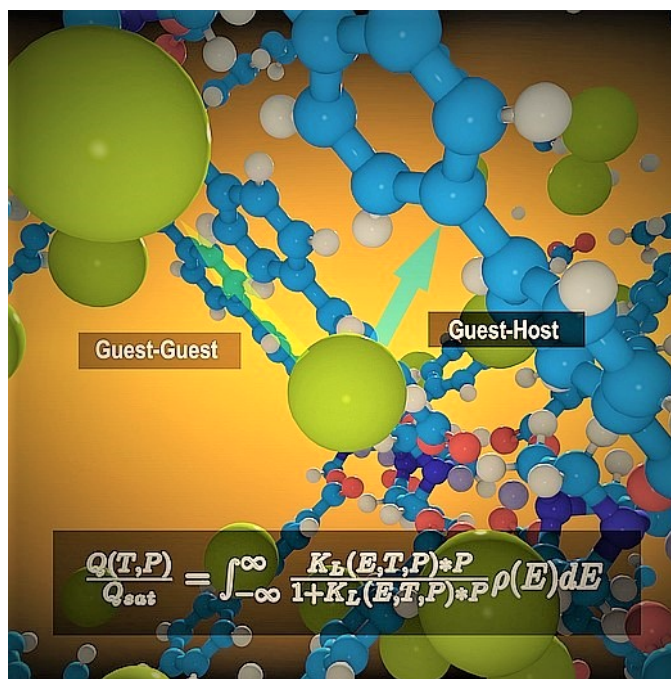
[2] Ziebel, M. E.; Darago, L. E.; Long, J. R. *J. Am. Chem. Soc.* **2018**, *140*, 3040-3051.

## Fast and Accurate Prediction of Hydrogen Adsorption in Nanoporous Materials

Arun Gopalan, Benjamin Bucior, N. Scott Bobbitt, and Randall Q. Snurr

Chemical and Biological Engineering, Northwestern University

We present a fast and accurate, semi-analytical method for predicting hydrogen adsorption in nanoporous materials. For any temperature and pressure, the adsorbed amount is calculated as an integral over the energy density of adsorption sites (guest host interactions) plus an average guest-guest term. The guest-host interaction energy is calculated using a classical force field with hydrogen modelled as a single-site probe. The guest-guest interaction energy is approximated using an average coordination number, which is regressed using Gaussian Process Regression (GPR). Local adsorption at each site is then modelled using a Langmuir isotherm, which when weighted with its probability density gives an accurate description of hydrogen adsorption. The method is tested on 933 metal-organic frameworks (MOFs) from the Computation-Ready Experimental (CoRE) MOF database at 77 K from to 100 bar, and the results are compared against GCMC predictions. To demonstrate the utility of the method, we calculated hydrogen adsorption isotherms for 12,914 existing MOF structures, at two different temperatures at a speed about 100 times that of GCMC simulations and analyzed the results. We found 13 MOFs with predicted deliverable capacities exceeding the DOE target of 50 g/L for adsorption at 100 bar, 77 K and desorption at 5 bar, 160 K.



**Publication:** Gopalan, A., Bucior, B. J., Bobbitt, N. S., & Snurr, R. Q. (2019). Prediction of hydrogen adsorption in nanoporous materials from the energy distribution of adsorption sites. *Molecular Physics*, (in press). <https://doi.org/10.1080/00268976.2019.1658910>.

**Software:** <https://github.com/snurr-group/pyIsoP>

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### **Huzinaga WF-in-DFT Embedding for MOFs**

Daniel Graham, Dhabih Chulhai, and Jason Goodpaster

Department of Chemistry, University of Minnesota-Twin Cities

Quantum embedding methods provide a strategy for performing localized highly accurate calculations on chemical systems while not incurring high cost computational scaling for the full system. Dividing a system into subsystems that are absolutely localized -- described by only the basis functions of the subsystem atoms -- can significantly reduce computational calculation time. The Huzinaga projection operator based absolute localization wavefunction embedded in density functional theory (WF-in-DFT) embedding methods match full system WF energy differences across a diverse test set. While our method requires very simple user input, several metrics may be used to determine how to divide systems into embedding subsystems. We have studied large metal organic framework (MOF) cluster models, specifically gas adsorption on MOF-74 variants. Our results indicate good agreement with full system WF methods, while incurring a fraction of the computational cost. Insights gained from embedding studies on MOFs could be used to guide experimental design and help reduce the number of candidates from MOF screening studies.

## Machine Learning Protocol Development for Automatic Active Space Selection in Multiconfigurational Self-Consistent Field Methods

WooSeok Jeong<sup>a</sup>, Samuel J. Stoneburner<sup>a</sup>, Ruye Li<sup>a</sup>, Andrew Walker<sup>b</sup>, Roland Lindh<sup>c</sup>, and Laura Gagliardi<sup>a</sup>

<sup>a</sup>Department of Chemistry, Minnesota Supercomputing Institute, and Chemical Theory Center, University of Minnesota-Twin Cities

<sup>b</sup>Department of Computer Science and Engineering, University of Minnesota-Twin Cities

<sup>c</sup>Department of Chemistry, Uppsala University

Multiconfigurational self-consistent field (MCSCF) methods are used for investigating the electronic structure of strongly correlated systems and chemical processes, which are not fully approachable for DFT calculations. One of the issues for the methods is that the appropriate selection of the active space, in which all possible electron configurations are considered, is not always obvious although it is critical for obtaining accurate results [1]. For automatic active space selection, a machine learning (ML) protocol is developed. As a first step, we have focused on the bond dissociation of neutral main group diatomic systems. Here, our strategy adopted a classification ML model to predict whether the given CASSCF result would be good or bad in terms of obtaining relatively good dissociative properties such as bond dissociation energy, equilibrium bond length, and vibrational constants. By testing CASSCF results at different internuclear distances for possible active space selections, one could identify which active space would be the best choice among the tested active spaces. For generation of raw data, complete active space self-consistent field (CASSCF) with second-order perturbation theory (CASPT2) calculations were performed with various active spaces. The internuclear distance, the number of active electrons/orbitals, occupation numbers, and molecular orbital (MO) coefficients are vectorized as features for training the classifier. Labeling of the features was automatized via comparisons of potential energy curves obtained by the simulations and theory/experimental data. The classification ML model was developed using the XGBoost (eXtreme Gradient Boosting), a decision tree based boosting algorithm [2]. We observed that the prediction performance of the developed ML model for unseen, test diatomic system strongly depends on which diatomic system(s) is used for the training set. This indicates there is a correlation between diatomic systems with respect to the prediction of good active space for the dissociation problem. Based on the correlation information, the ML model can be used to predict correctly good active spaces for systems that are not in the training set.

### References

- [1] Veryazov, V.; Malmqvist, P. Å.; Roos, B. O. How to Select Active Space for Multiconfigurational Quantum Chemistry? *Int. J. Quantum Chem.* **2011**, 111 (13), 3329–3338.
- [2] Chen, T.; Guestrin, C. XGBoost: A Scalable Tree Boosting System. In Proceedings of the 22Nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining; KDD '16; ACM: New York, NY, USA, **2016**; pp 785–794.

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## **Generation of Machine Learning Potentials for Small Molecule Homogeneous Systems Using Neural Networks**

Andrew Johannesen and Jason Goodpaster

Department of Chemistry, University of Minnesota-Twin Cities

Force fields offer a method of determining a system's potential energy with little computational cost and are especially useful in visualization and prediction of a system's behavior. They are limited in their accuracy due to their low-cost constraint, and work in recent years has offered the machine learning potential as an alternative with improved accuracy while retaining a low computational cost. Since machine learning potentials can construct a direct functional relationship between atomistic spatial configurations and energies, their accuracy is primarily limited by the quality of training data, yielding results commensurate with the training data's level of theory.

The objective of this work is to produce a series of machine learning potentials for homogeneous systems of small molecules using neural networks while outlining the considerations necessary for a generalizable method of machine learning potential creation for arbitrary closed shell small molecules. Potentials have been created for carbon dioxide, and molecular nitrogen, yielding potentials able to accurately reproduce select density functional theory calculations at a fraction of the cost. In the creation of these potentials, a series of necessary considerations for the generalized production of machine learning potentials for small molecules were uncovered.

Future work includes the augmentation of existing potentials with electronic structure data to improve each's level of accuracy, the production of potentials for additional target molecules, and the formulation of a generalized method to produce machine learning potentials for small molecules. In addition to improving training data and expanding the current potential library, tuning of neural network parameters and exploring alternative machine learning methods to optimize interpolation capacity are goals of interest.

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## **Quantum Mechanical Studies of Nanoporous Materials**

Britta Johnson and Nandini Ananth

Department of Chemistry and Chemical Biology, Cornell University

Several of the unique characteristics shown by nanoporous materials are thought to be of quantum mechanical origin. For instance, nuclear zero-point energy is expected to play a significant role in accurately determining gas separation, adsorption, and diffusion in systems where the pore size and the molecular diameter are similar in magnitude. We employ path integral molecular dynamics (PIMD) methods to model these systems because it scales classically with system size but still captures quantum effects like zero-point energy and tunneling. Specifically, we compare the classical and quantum energetic barriers to molecular insertion and molecular diffusion for ethane and ethene in a series of zeolites which the Siepmann group has found to be highly selective for one adsorbate over the other.

We are also studying charge transfer reactions in nanoporous materials that require the use of quantum methods to obtain accurate rates and provide insights into the mechanism at the atomistic level. We are developing and implementing approximate quantum mechanical path integral methods: ring polymer molecular dynamics (RPMD) and mean-field ring polymer molecular dynamics (MF-RPMD) for multi-state systems. Target systems for our reaction rate calculations include MOFs currently under investigation by Long/Gagliardi groups and the Goodpaster/Marinescu groups.



## Molecular simulations and machine learning for multicomponent adsorption: BTEX separation with zeolite membranes

Tyler R. Josephson<sup>a</sup>, Yangzesheng Sun<sup>a</sup>, Evgenii O. Fetisov<sup>a,c</sup>, J. R. Johnson<sup>d</sup>, Benjamin A. McCool<sup>d</sup>, Michael Tsapatsis<sup>b,e</sup>, and J. Ilja Siepmann<sup>a,b</sup>

<sup>a</sup> Department of Chemistry and Chemical Theory Center, University of Minnesota

<sup>b</sup> Department of Chemical Engineering and Materials Science, University of Minnesota

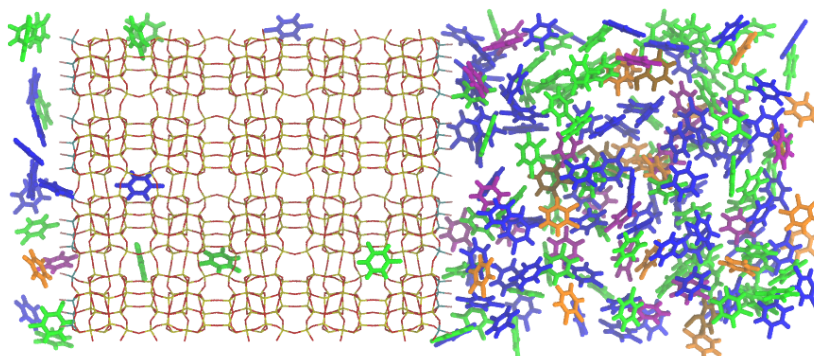
<sup>c</sup> Pacific Northwest National Lab

<sup>d</sup> Corporate Strategic Research, ExxonMobil Research and Engineering

<sup>e</sup> Department of Chemical and Biomolecular Engineering, John Hopkins University

Separation of *p*-xylene from mixtures of benzene, toluene, ethylbenzene, and xylenes (BTEX) is a critical industrial process, identified as one of “seven chemical separations to change the world” [1]. Membranes that permit selective transport of *p*-xylene, but not its isomers, *o*-xylene, *m*-xylene, and ethylbenzene, could dramatically improve the efficiency of *p*-xylene production. Zeolite membranes are stable under the high temperatures and pressures of the catalytic process; membranes synthesized with the MFI framework enable high selectivity and flux for *p*-xylene separation when tested at pressures < 1 bar and at temperatures up to 425 K [2]. However, at high temperatures and pressures, adsorption of aromatics into zeolite membranes saturates the pores, shutting down transport.

Process design of a *p*-xylene-selective membrane reactor requires knowledge of adsorption and transport through the membrane across a range of industrial process conditions. To address the question of multicomponent adsorption into MFI zeolite at elevated temperatures and pressures, we performed high-throughput Monte Carlo simulations in the Gibbs ensemble to predict BTEX adsorption across the expansive “process space” of potential operating conditions. The transferrable potentials for phase equilibria (TraPPE) force field was developed to accurately predict vapor-liquid coexistence curves for alkyl-substituted aromatics. Then, unary and multicomponent adsorption isotherms and fluid phase properties are predicted across a multidimensional composition space, and from liquid, vapor, and supercritical phases. These simulations provide individual data points that are used to fit an artificial neural network, which provides a single, self-consistent, continuous, and differentiable function describing the properties of both the fluid and adsorbed phases across the full range of realistic process conditions.



### References

- [1] D.S. Sholl and R.P. Lively, *Nature*, 532, **2016**, 436-437.
- [2] M.Y. Jeon, et al. *Nature*, 543, **2017**, 690-694.

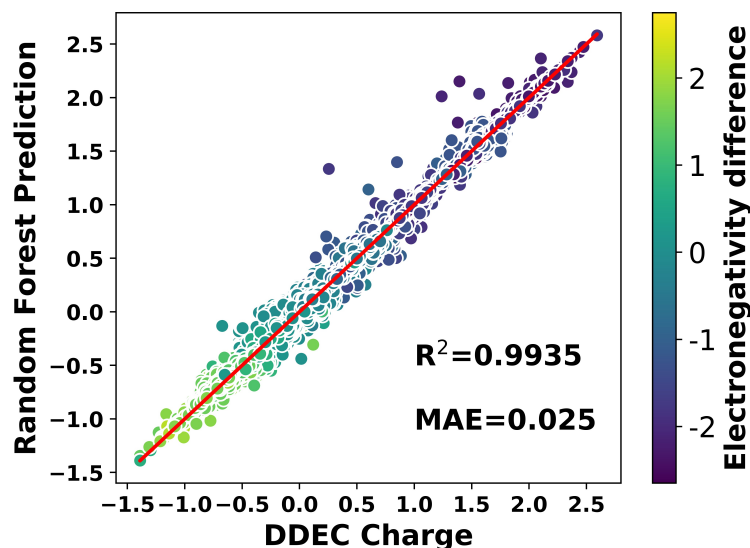
## High-Quality Partial Atomic Charges for MOFs from Machine Learning

Srinivasu Kancharlapalli<sup>a,b</sup>, Arun Gopalan<sup>a</sup>, and Randall Q. Snurr<sup>a</sup>

<sup>a</sup>Department of Chemical and Biological Engineering, Northwestern University

<sup>b</sup>Theoretical Chemistry Section, Bhabha Atomic Research Centre, Mumbai, India

High-throughput screening (HTS) using grand canonical Monte Carlo simulations is a useful strategy for identifying metal-organic frameworks (MOFs) for adsorption and separation applications. However, accurate partial atomic charges are required to capture the interactions between the MOF and the adsorbates during HTS, especially when the adsorption involves polar molecules like water and CO<sub>2</sub>. Although DFT based methods such as Density Derived Electrostatic and Chemical (DDEC) [1] atomic charges and repeating electrostatic potential extracted atomic (REPEAT)[2] charges are known to be quite reliable, the high-computational cost associated with these methods make them impractical in the screening of large material databases. In this work, we used a Random Forest machine learning model involving a list of features that represent both the elemental properties and the local atomic environment to predict the partial atomic charges in MOFs accurately. Our Random Forest model is trained and tested on a collection of about 380,000 partial atomic charges calculated using the DDEC method on a subset of 4700 MOFs from the CoRE-MOF 2019 All Solvent Removed (ASR) database [3]. The figure shows that the partial atomic charges predicted by Random Forest agree very well with the DFT derived DDEC charges. Good correlation is observed between the partial atomic charge and the difference between the electronegativity of the atom and the average electronegativity of the coordinated atoms.



**Figure:** Parity between the partial atomic charges calculated using DDEC and that from machine learning (ML) for all the datapoints in the testing set. The color indicates the difference between the electronegativity of the atom and the average electronegativity of the coordinated atoms.

### References

1. Manz, T. A.; Sholl, D. S. *J. Chem. Theory Comput.* **2010**, *6*, 2455–2468.
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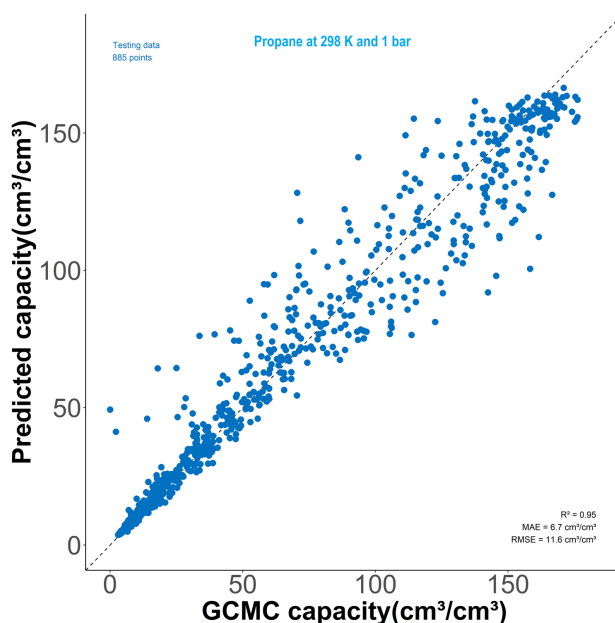
## Machine learning using the guest/host energy histogram to predict alkane adsorption and xenon/krypton separation

Zhao Li, Benjamin Bucior, N. Scott Bobbitt, Randall Snurr

Department of Chemical and Biological Engineering, Northwestern University, Evanston, IL

Machine learning, as it gains more and more usefulness in computational researches, has been successfully used to study nano-porous materials such as zeolites and metal-organic frameworks (MOFs). Recently, Bucior et al. published a study<sup>1</sup> using histograms of the guest/host energy as features for LASSO, which is a linear regression machine learning method, to investigate and predict the top candidates for hydrogen and methane storage in MOFs.

In this work, we refined the energy histogram methodology and extended it to longer alkanes like ethane, propane, and n-hexane. Energy histograms are now automatically aggregated without pre-determined bin sizes such that if a range of energy values has more counts, it is represented with more bins in the histogram. To test our new methodology, we performed grand canonical Monte Carlo (GCMC) simulations for materials from ToBaCCo MOF sets<sup>2</sup>. Both linear and non-linear models such as LASSO and Random Forest were used to perform regression. We find that as the size of the alkane increases, non-linearity in the model increases and thus non-linear regression methods must be used. We also tested additional new features to compensate information loss when constructing histograms from the three-dimensional energy grids. Additionally, the new algorithm shows robustness when predicting selectivity for Xe/Kr separation.



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**Spin-State Ordering in Metal-Based Compounds  
Using the Localized Active Space Self-Consistent Field Method**

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Quantitatively accurate calculations for spin-state ordering in transition-metal complexes typically demand a robust multiconfigurational treatment. The poor scaling of such methods with increasing size makes them impractical for large, strongly correlated systems. Density matrix embedding theory (DMET) is a fragmentation approach that can be used to specifically address this challenge. The single-determinantal bath framework of DMET is applicable in many situations, but it has been shown to perform poorly for molecules characterized by strong correlation when a multiconfigurational self-consistent field solver is used. To ameliorate this problem, the localized active space self-consistent field (LASSCF) method was recently described. In this work, LASSCF is applied to predict spin-state energetics in mono- and di-iron systems, and we show that the model offers an accuracy equivalent to that of CASSCF but at a substantially lower computational cost. Performance as a function of basis set and active space is also examined.

## Theoretical Insights into Solvent Effects on Sugar Transformation Chemistry in Modified UiO-66

Roshan Ashokbhai Patel<sup>a,b</sup>, Matheus Dorneles De Mello<sup>a</sup>, Tyler R. Josephson<sup>b</sup>, Michael Tsapatsis<sup>a,c</sup>,  
J. Ilja Siepmann<sup>a,b</sup>, and Matthew Neurock<sup>a</sup>

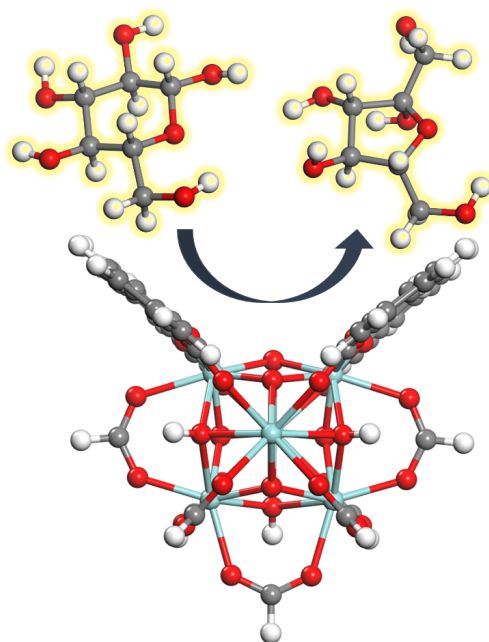
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Solvents are used in many industrial processes and play a pivotal role in aiding many catalytic transformations by influencing the reaction rates and mechanisms. The rates and selectivities of acid-catalyzed transformations, for example, can be significantly improved by changing solvents. Nanoporous catalysts such as metal-organic frameworks (MOFs) can offer larger pore sizes that can aid in configuring solvent environments to stabilize transition states and promote catalytic transformations. In this work, we focus on acid-catalyzed transformations involved in the conversion of glucose to fructose over modified UiO-66 in presence of different alcohol solvents.

Specifically, we examine different pathways for glucose-to-fructose isomerization and the side reaction involving the acetalization reaction of glucose with alcohol as well as the influence of different alcohol solvents (methanol and propanol) using density functional theory (DFT) and a cluster-based UiO-66 model. Preliminary studies show that propanol promotes the rate-determining hydride shift step in glucose isomerization more than methanol whereas a lower barrier is seen for the acetalization reaction of glucose with methanol than propanol. This can be attributed to their different hydrogen-bonding and solvation abilities as well as alkoxide basicities which affect the fructose selectivity in different solvents. Further investigation with other solvents can help identify potential solvents/mixtures of solvents which can aid in driving these acid-catalyzed transformations.

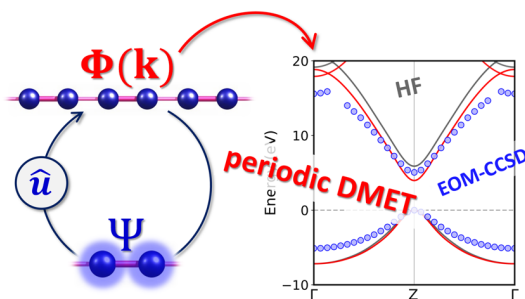


## Electronic structure of solid-state materials with density matrix embedding theory

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We extended density matrix embedding theory (DMET) to periodic systems. In periodic DMET, electron correlation can be captured by means of a local impurity model using various wave function methods. The method is able to describe not only the ground-state energy but also the quasiparticle band picture via the real space-momentum space implementation. The performance of periodic DMET was tested on a series of one-dimensional solids, such as hydrogen chain, LiH, and polyyne. Our results show that DMET agrees well with other many-body techniques. We anticipate that periodic DMET can be a promising first principle technique for materials with strongly correlated electrons.

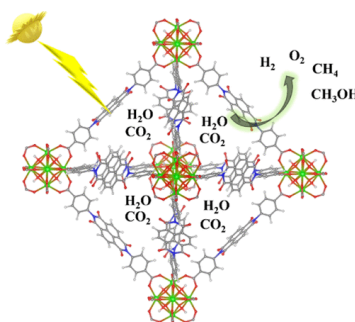


## Metal-Organic Frameworks for Photocatalytic and Optoelectronic Applications

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Metal organic frameworks (MOFs) are rapidly evolving into an important class of materials due to their inherent structural diversity and their advantageous application for diverse purposes including gas storage and separation, catalysis, chemical sensing, and optical applications.<sup>1-3</sup> Light-harvesting MOFs have the potential to be exploited for the design of 3<sup>rd</sup> generation devices for optoelectronic applications as well as selective photocatalysts.<sup>3</sup> However, detailed understanding of the nature of charge transport mechanisms in MOFs is vital to the design of solar-energy materials that are based on them. Using density functional theory, we have rationalized the photophysics and electron-transfer processes in two different classes of MOFs, namely, UiO-NDI and porphyrin-containing MOFs incorporating C<sub>60</sub> as a guest (DA and F-MOF, specifically). Our calculations suggest that UiO-NDI MOF should be an excellent platform for designing efficient MOF-based photocatalysts for water splitting and CO<sub>2</sub> reduction.<sup>4</sup> In addition, charge-transfer interactions between donor-acceptor conjugates in the porphyrin-based MOFs incorporating C<sub>60</sub> are predicted to accelerate charge separation processes that should lead to high electrical conductivity. Our results provide insights that should stimulate further investigations aimed at the development of clean and sustainable MOF-derived energy materials.



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## Gold nanoparticles in the NU-1000 metal organic framework: Structures and O<sub>2</sub> activation

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Well-dispersed gold nanoparticles (AuNPs) on a solid support with control of particle size is a goal for heterogeneous catalysis. Experiment has shown that the Zr-based metal-organic framework NU-1000 can be used as both a size-defining template and a support for the growth of AuNPs growth. These AuNPs have shown to be catalytically competent for reduction reactions and could be effective for selective oxidative catalysis. A key step in gold-catalyzed oxidations is the activation of O<sub>2</sub>, which has not yet been studied within a MOF. In this work, the energies of isomeric Au<sub>13</sub> and Au<sub>38</sub> NPs confined in NU-1000 have been characterized together with an examination of O<sub>2</sub> activation thereupon.

In particular, periodic density functional theory calculations were performed with the AuNPs incorporated into the triangular pores of NU-1000, and O<sub>2</sub> binding was studied for the most stable conformations. We find that the well-studied Au<sub>38</sub> cuboctahedron is not stable inside the triangular pore, but instead relaxes to more stable and less symmetric structures having 5- or 4-atom cores, which are similar to geometries found to be at low energy when in isolated form in a previous study. These NPs have singlet spin ground states. Within the triangular pore, O<sub>2</sub> binding on exposed gold surfaces is sensitive to the gold surface arrangement and the overall spin. Tuning the gold surfaces through gold-linker interactions could be a one way to optimize the activity of gold catalysts within MOFs.



## Fingerprinting all-silica zeolites for hydrogen storage using meta-learning

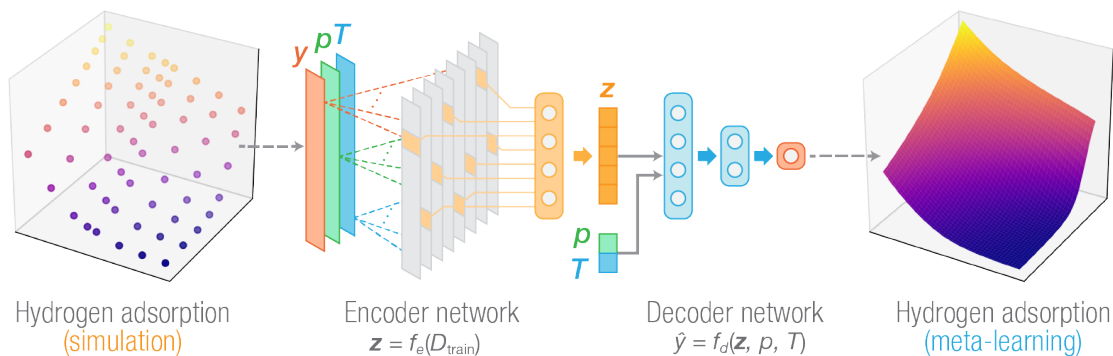
Yangzesheng Sun<sup>a</sup>, Robert F. DeJaco<sup>a,b</sup>, Matthias Thommes<sup>c</sup>, Martin Hartmann<sup>c</sup>, and J. Ilja Siepmann<sup>a,b</sup>

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Adsorbent materials store large amounts of hydrogen and do not require very high pressures, making them especially suitable for fuel cell vehicles. The hydrogen storage performance of nanoporous materials are typically probed at very low temperatures like 77 K, since equilibrium loading is larger at lower temperatures. However, our molecular simulation results reveal that higher temperatures may yield higher working capacities for the storage of hydrogen. In this work, we developed a meta-learning neural network which simultaneously predicts the adsorption for multiple materials at multiple pressures and temperatures. The network compresses the entire  $(p, T)$  adsorption surface into a fingerprint vector and predicts the adsorption more accurately than conventional isotherm fitting methods. From Monte Carlo simulations performed on all-silica zeolites in the International Zeolite Association (IZA) database, we applied the meta-learning method to probe the optimal hydrogen storage temperature for each zeolite. The highest optimal temperature among these zeolites were found to be around 140 K. We also discovered that zeolites with high optimal temperatures are closer in the fingerprint space and have high isosteric heat of adsorption at the zero-loading limit. Another advantage of our machine learning approach is that it is more robust to erroneous results from sporadic failed simulations, making it particularly suitable for high-throughput discovery of nanoporous materials.



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**Prediction model for Adsorption in Metal-Organic Frameworks Developed by Machine Learning  
Algorithm: Separation of Near-Azeotropic Species**

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School of Chemical & Biomolecular Engineering, Georgia Institute of Technology

Adsorption-based process can energy-efficiently separate mixtures by suitable adsorbent materials. Discovering the mixture-specific adsorbents among millions industry-relevant molecules is infeasible in experiments. In this study, we provide one prediction model for adsorption in metal-organic frameworks (MOFs) being explored with machine learning algorithm, using large number of adsorption isotherms generated by atomistic simulations for a diverse set of adsorbates and adsorbents. We introduce a new robust procedure to generalize thousands of descriptors that already known from molecular systems to crystalline nanoporous materials. Those descriptors enable machine learning approaches to efficiently and accurately prediction single component adsorption isotherms for diverse collections of molecules and MOFs. The prediction model developed is further used for predicting the separation of near-azeotropic species.

## Automated Metal-Organic Framework Discovery Platform for Clean Energy Applications

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Metal-Organic frameworks (MOFs) are crystalline, nanoporous materials composed of (in)organic nodes connected by organic linkers. Because of their highly tunable structure, high porosity, and large internal surface area, MOFs are of great interest for various applications such as catalysis, gas separation, and gas storage. The multitude of nodes, linkers, and functional groups can be combined to form a vast array of plausible MOF structures. The chemical space of all possible MOFs is far too large to thoroughly sample using brute force; therefore, we must turn to automated search methods to identify promising candidates tailored for a specific application. We designed a hybrid variational autoencoder (VAE) for the automated design of novel MOFs and trained it with known MOF structures. MOF structures were automatically decomposed into their building block sequence (linker+node+topology), and a graph-based junction-tree pre-VAE was used to learn and predict new linkers and nodes while a sequence-based VAE is used to learn and predict new building block sequences with the optimization guided by the calculated properties of previously generated MOFs. We now have a database consisting around 15 million valid MOF structures and currently we are aiming at clean energy applications including gas separation and storage. Performance properties of our top candidates are being validated using computational approaches and we also are seeking assistance on experimental synthesis and measurement. In the future, we will utilize the hybrid VAE and for more clean energy related applications, train the hybrid VAE with corresponding properties and predict MOFs with improved performance.

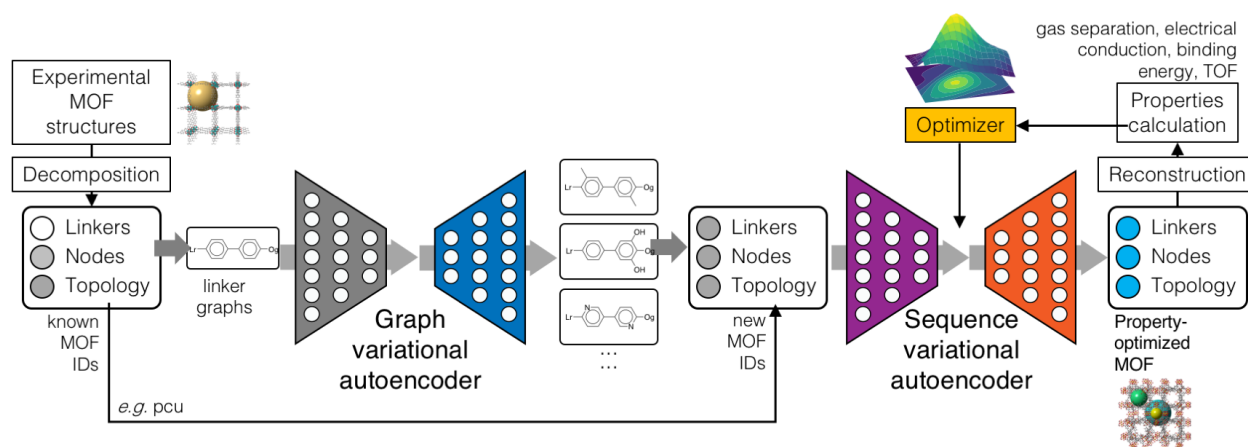


Figure 1. Illustration of the Automated Metal-Organic Framework Discovery Platform.

## A 3D Convolutional Neural Network based Variational Autoencoder for Gas Storage Prediction of Zeolites

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Zeolites have high internal surface area and internal porosity, which makes them good candidates for gas and liquid storage applications. While experimental and computational determination of the properties of zeolites can be time and resource consuming, machine learning approaches can be used to accelerate the process by revealing the underlying intrinsic correlations between zeolite structures and making property predictions. In this project, we represented all the known zeolite structures with their potential grids and fed them to an as-built 3D convolutional neural network (CNN) based variational autoencoder (VAE). Considering that state-of-the-art zeolites are pretty limited (~300) with an insufficient amount of structural features can be passed to the CNN network, we enriched our feeding database with potential grids from other common oxide (~10k) crystal structures obtained from the Inorganic Crystal Structure Database (ICSD).<sup>1</sup> We are now generating the potential grids for all the added normal oxides and the CNNVAE will be trained with all these grids and zeolite properties computed. Our CNNVAE will be capable to make predictions of zeolite properties and we will also try to identify the critical structural features of zeolite structures with superior performance, offering design guidance for the future development of novel zeolites.

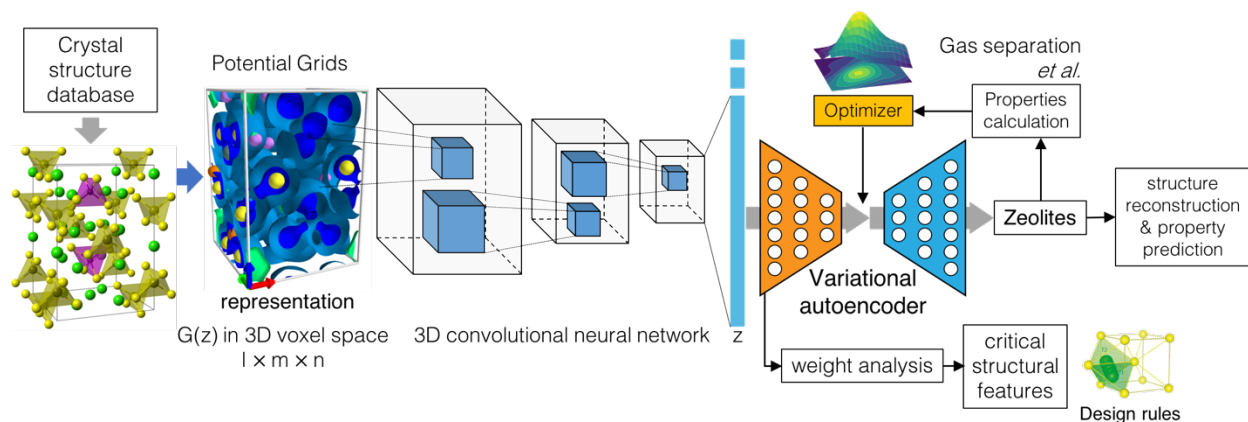


Figure 2. Illustration of the 3D convolutional neural network based VAE for the design of novel Zeolites.

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## Energy Storage, Gas Separations, and Charge Transport in Redox-Active Metal–Organic Frameworks

Michael Ziebel<sup>a</sup>, Julia Oktawiec<sup>a</sup>, Jesse Park<sup>a</sup>, Lucy Darago<sup>a</sup>, Carlo Gaggioli<sup>c</sup>, Jenny Vitillo<sup>c</sup>, Brianna Collins<sup>c</sup>,  
Jingyun Ye<sup>c</sup>, Donald Truhlar<sup>c</sup>, Jason Goodpaster<sup>c</sup>, Laura Gagliardi<sup>c</sup>, and Jeffrey Long<sup>a,b,d</sup>

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The ability to control electronic structure in metal–organic materials through precise modification of metal, ligand, and topology enables a diverse range of chemical and materials properties which has led to their use across a wide range of applications. The incorporation of redox-active metals or ligands into these materials facilitates post-synthetic modification of their electronic structure, while also opening new applications which utilize this redox chemistry. Energy storage devices rely on cathode materials which can accept and release large amounts of charge at high potentials. The combination of redox-active metals and ligands in metal–organic frameworks could enable storage capacities which surpass those of traditional oxide-based cathodes. An iron-semiquinoid framework, which utilizes a combination of metal- and ligand-centered redox processes, shows great promise to this end. O<sub>2</sub>/N<sub>2</sub> separations are made challenging by the similar polarizabilities and kinetic diameters of the two gases. Electron-rich frameworks can bind O<sub>2</sub> selectively through a redox-mediated process, but most frameworks bind O<sub>2</sub> too strongly (leading to irreversibility) or too weakly at room temperature. A cobalt-azolate framework which possesses excellent selectivity for O<sub>2</sub> due to its combination of an electron-rich metal center and a stabilizing hydrogen bonding site illustrates design principles required for performing this separation at high temperatures. Finally, the mechanism of charge transport in metal–organic materials is poorly understood, particularly the origins of localization in frameworks which are predicted to be metallic by band structure calculations. The use of high pressure in diamond anvil cells can begin to differentiate between phonon-driven effects and orbital-driven effects. The high pressure characterization of a highly conductive iron triazolate framework will be discussed. Overall, we will illustrate the use of redox-active frameworks across multiple applications and will discuss the implications of local electronic structure changes on bulk material properties.

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\* 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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