

# NMGC

nanoporous materials genome center



## 2020 ALL-HANDS MEETING

OCTOBER 8 - 9, 2020

UNIVERSITY OF MINNESOTA

# TABLE OF CONTENTS

PROGRAM.....Page 1

POSTER SESSIONS .....Pages 2-4

ABSTRACTS.....Pages 5-32  
listed by Poster Session, in alphabetical order

ATTENDEE LIST.....Pages 33-34

All Times Central

**Thursday, October 8, 2020**

- 8:30a – 8:35a Welcome
- 8:35a – 8:55a Overview
- 8:55a – 9:25a **Alan Aspuru-Guzik**  
Artificial Intelligence for MOF design
- 9:25a – 9:55a **Randall Snurr**  
Development of Tools for Design and High-throughput Computational Screening of MOFs for Adsorption Applications
- 9:55a – 10:05a *Break*
- 10:05a – 10:35a **Coray Colina**  
Advances for Predictive Modeling of Adsorption in Disorder Nanoporous Materials
- 10:35a – 11:05a **David Sholl**  
Predicting Adsorption Selectivity for Diverse Chemical Mixtures
- 11:05a – 11:35p **Ilja Siepmann**  
Machine learning, high-throughput simulations, and first principles calculations for chemical separations and transformations
- 11:35a – 11:45a *Break*
- 11:45p – 12:15p **Maciej Haranczyk**  
Structure characterization, new descriptors and datasets
- 12:15p – 12:45p **Nandini Ananth**  
Characterizing porous materials with electronic structure and atomistic path integral simulations

**Friday, October 9, 2020**

- 8:30a – 9:00a **Smaranda Marinescu**  
Conductive Dithiolene-Based MOFs for H<sub>2</sub> Evolution
- 9:00a – 9:30a **Laura Gagliardi**  
Electronic Structure Theories for Porous Materials Properties
- 9:30a – 9:45a *Break*
- 9:45a – 10:15a **Jason Goodpaster**  
Method development and application to Metal Organic Frameworks: Quantum Embedding and Machine learning
- 10:15a – 10:45a **Donald Truhlar**  
Highlights of NMGC Research in the Truhlar Group in the Past Year
- 10:45a – 11:00a *Break*
- 11:00a – 12:00p Scientific Advisory Board Meeting
- 12:00p – 1:00p Principal Investigators Meeting
- 1:00p – 2:00p Poster Session A
- 2:00p – 2:15p *Break*
- 2:15p – 3:15p Poster Session B
- 3:15p – 3:30p *Break*
- 3:30p – 4:30p Poster Session C
- 4:30p – 5:30p Executive Committee Meeting

**Poster Session A, 1:00p – 2:00p**

Keying Chen

Cu[Ni(2,3-pyrazinedithiolate)<sub>2</sub>] Metal-Organic Framework for Electrocatalytic Hydrogen Evolution

Brianna Collins

Itinerant ferromagnetism in a mixed-valent metal-organic framework: A DFT Perspective

Riki Drout

Isothermal Titration Calorimetry to Explore the Parameter Space of Organophosphorus Agrochemical Adsorption in MOFs

Carlo Alberto Gaggioli & WooSeok Jeong

Using Active Machine Learning Protocol to Accelerate Excited State Multireference Calculations of Organic Molecules

Subhadip Goswami & Debmalya Ray

Engineering Electrical Conductivity of Hexa-Zr(IV) Metal-Organic Frameworks

Matthew R. Hermes

State averaging and state interaction in LASSCF

Britta Johnson

Towards Atomistic Simulations of Nonadiabatic Reaction Dynamics

Andrew Rosen

Machine Learning the Quantum-Chemical Properties of Metal–Organic Frameworks with a New Electronic Structure Database

Dai Tang

Predicting Separation of Near-Azeotropic Mixtures by a Machine Learning Model

**Poster Session B, 2:15p – 3:15p**

Dylan Anstine

Evaluating Adsorption Space for Polymers of Intrinsic Microporosity with Diverse Adsorbate Species

Xiaozhe Fan

Adsorption mechanism of para-xylene in the Ba-exchanged faujasite zeolite

Andrew Johannesen

Reactive Machine Learning Potential Models for the NO Formation Reaction

Roshan Patel

Monte Carlo simulations to understand solvent adsorption in UiO-66

Hung Pham

Materials Modelling using Density Matrix Embedding Theory

Huilong Shao

Computational investigation on the reaction mechanism of Co(II)-MFU-4L catalyzed 1,3-butadiene polymerization

Kaihang Shi

MOFdb: An accessible online database of computational adsorption data for nanoporous materials

Yangzesheng (Andrew) Sun

Generative machine learning for the spatial distribution of adsorption in all-silica zeolites

**Poster Session C, 3:30p – 4:30p**

Saumil Chheda

Solvent adsorption in multivariate MOFs using Monte Carlo simulations

Alexander Demidov

Dynamics of PEO/PP melts on a silicalite nanosheet by atomistic simulations

Daniel Graham

Huzinaga WF-in-DFT Embedding for Complex Open-shell Systems

Quin Hu

Neural Network Potentials for Bond Dissociation

Zhao Li

Machine Learning Using Host/Guest Energy Histograms to Predict Adsorption in Metal-Organic Frameworks: Application to Chain Molecules and Mixtures

Riddhish Pandharkar

Spin state analysis using pair density functional theory using localized active space wavefunctions

Michael Ziebel

Understanding Covalency and Redox-Chemistry in Metal–Organic Frameworks

SCIENTIFIC ADVISORY BOARD		
Robert Giraud	The Chemours Company	Scientific Advisory Board
Joachim Sauer	Humboldt University	Scientific Advisory Board
Cathy Tway	Johnson Matthey	Scientific Advisory Board
SENIOR PERSONNEL		
EXECUTIVE COMMITTEE		
Ilja Siepmann	University of Minnesota	Director Principal Investigator
Donald Truhlar	University of Minnesota	Deputy Director Thrust C Representative* Co-Investigator
Alán Aspuru-Guzik	University of Toronto	Thrust A Representative* Co-Investigator
Smaranda Marinescu	University of Southern California	Experimental Integration Co-Investigator
Randall Snurr	Northwestern University	Thrust B Representative* Co-Investigator
INVESTIGATORS		
Coray Colina	University of Florida	Co-Investigator
Christopher Cramer	University of Minnesota	Co-Investigator
Omar Farha	Northwestern University	Co-Investigator
Laura Gagliardi	University of Minnesota	Co-Investigator
Jason Goodpaster	University of Minnesota	Co-Investigator
Maciej Haranczyk	IMDEA Materials	Co-Investigator
Joe Hupp	Northwestern University	Co-Investigator
Jeffrey Long	University of California, Berkeley	Co-Investigator
David Sholl	Georgia Institute of Technology	Co-Investigator
JUNIOR RESEARCHERS		
Dylan Anstine	University of Florida (Colina)	Graduate Student
Suman Bhaumik	University of Minnesota (Truhlar)	Graduate Student
Keying Chen	University of Southern California (Marinescu)	Graduate Student
Haoyuan Chen	Northwestern (Snurr)	Research Associate
Saamil Chheda	University of Minnesota (Gagliardi/Siepmann)	Graduate Student
Brianna Collins	University of Minnesota (Goodpaster)	Graduate Student
Alexander Demidov	University of Florida (Colina)	Graduate Student
Riki Drout	Northwestern University (Farha)	Graduate Student
Jiaxin (Dawn) Duan	Northwestern University (Farha/Hupp)	Graduate Student
Xiaozhe Fan	University of Minnesota (Truhlar)	Visiting Researcher
Carlo Alberto Gaggioli	University of Minnesota (Gagliardi)	Postdoctoral Researcher
Arun Gopalan	Northwestern (Snurr)	Graduate Student
Subhadip Goswami	Northwestern (Farha/Hupp)	Research Associate
Daniel Graham	University of Minnesota (Goodpaster)	Graduate Student
Sai Govind Hari Kumar	University of Toronto (Aspuru-Guzik)	Graduate Student
Matthew R. Hermes	University of Minnesota (Gagliardi)	Postdoctoral Researcher
Quin Hu	University of Minnesota (Goodpaster)	Graduate Student

JUNIOR RESEARCHERS, CONTINUED....		
WooSeok Jeong	University of Minnesota (Gagliardi)	Postdoctoral Researcher
Andrew Johannesen	University of Minnesota (Goodpaster)	Graduate Student
Britta Johnson	Cornell University (Ananth)	Postdoctoral Researcher
Siriluk Kanchanakungwankul	University of Minnesota (Truhlar)	Graduate Student
Srinivasu Kancharlapalli	Northwestern University (Snurr)	Postdoctoral Researcher
Zhao Li	Northwestern University (Snurr)	Graduate Student
Jiaxin Ning	University of Minnesota (Truhlar)	Graduate Student
Riddhish Pandharkar	University of Minnesota (Cramer/Gagliardi)	Graduate Student
Roshan Patel	University of Minnesota (Siepmann/Tsapatsis)	Graduate Student
Thang Pham	Northwestern University (Snurr)	Graduate Student
Hung Pham	University of Minnesota (Gagliardi)	Graduate Student
Debmalya Ray	University of Minnesota (Gagliardi)	Graduate Student
Andrew Rosen	Northwestern University (Snurr)	Graduate Student
Huilong Shao	University of Minnesota (Cramer)	Postdoctoral Researcher
Thomas Sheridan	Northwestern University (Hupp)	Graduate Student
Kaihang Shi	Northwestern University (Snurr)	Postdoctoral Researcher
Ramanish Singh	University of Minnesota (Siepmann)	Graduate Student
Andrew Yangzesheng Sun	University of Minnesota (Siepmann)	Graduate Student
Dai Tang	Georgia Institute of Technology (Sholl)	Postdoctoral Researcher
Dihua Wu	University of Minnesota (Truhlar)	Postdoctoral Researcher
Zhenpeng Yao	University of Toronto (Aspuru-Guzik)	Postdoctoral Researcher
Dayou Zhang	University of Minnesota (Truhlar)	Graduate Student
Chen Zhou	University of Minnesota (Truhlar)	Postdoctoral Researcher
Michael Ziebel	University of California, Berkeley (Long)	Graduate Student

\* 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



## ACKNOWLEDGEMENT

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THE NANOPOROUS MATERIALS GENOME CENTER IS SUPPORTED BY THE  
U.S. DEPARTMENT OF ENERGY, OFFICE OF BASIC ENERGY SCIENCES,  
UNDER AWARD DE-FG02-17ER16362, AS PART OF THE COMPUTATIONAL  
CHEMICAL SCIENCES PROGRAM.