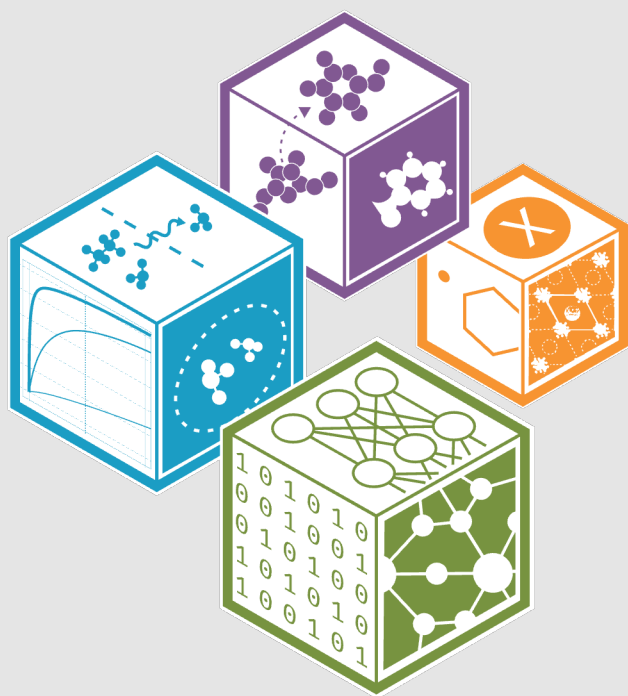


NMGC

nanoporous materials genome center

2022 All-Hands Meeting



APRIL 4 – APRIL 5, 2022

UNIVERSITY OF MINNESOTA

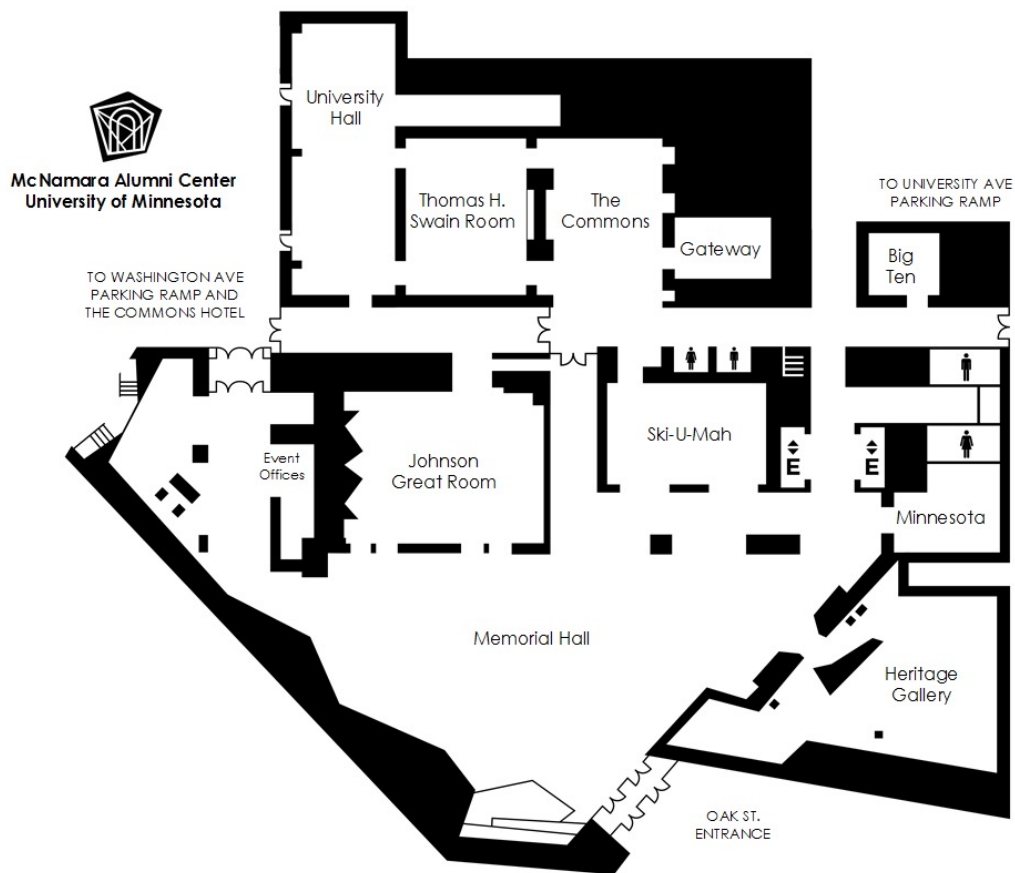
TABLE OF CONTENTS:

AGENDA Page 1

ZOOM INFORMATION..... Page 2

ABSTRACTS..... Pages 4 - 12
listed in alphabetical order by first author's last name

ATTENDEE LIST..... Pages 13 - 14



LOCATION

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

April 4 – April 5, 2022 | University of Minnesota

All events held in McNamara Alumni Center, Thomas Swain Room, unless otherwise noted

Monday, April 4, 2022

- 9:00a – 9:45a** **Registration opens, Continental Breakfast available**
- 9:45a – 10:00a Welcome & Overview
- 10:00a – 10:30a Jason Goodpaster
Advancements in Machine Learning and Quantum Embedding for Large Scale Simulations
- 10:30a – 11:00a Abhishek Mitra
Understanding Local Excitations in Solids and Surface Binding using Density Matrix Embedding Theory
- 11:00a – 11:20a** **Break**
- 11:20a – 11:50a Jingyun Ye
Computational Study of Oxygen Evolution Reaction Catalyzed by Bimetallic Metal Organic Frameworks
- 11:50a – 12:20p Siriluk Kanchanakungwankul
Selective partial oxidation of methane to methanol by Cu-ZIF-8
- 12:20p – 1:30p** **Boxed Lunch**
- 1:30p – 2:00p Saumil Chheda
N,N-dimethylformamide (DMF) adsorption in structurally flexible IRMOFs
- 2:00p – 2:30p Roshan Ashokbhai Patel
Predicting NH₃/N₂/H₂ separation performance of MFI zeolite nanosheet membranes at high temperature and pressure
- 2:30p – 3:00p Richard Shiery
Structure of Water in Faujasite
- 3:00p – 3:15p** **Group Photo**
- 3:15p – 3:45p** **Break**
- 3:45p – 4:15p Yangzesheng (Andrew) Sun
Understanding and Predicting Spatially-resolved Loading Surfaces of Nanoporous Materials
- 4:15p – 4:45p Thang Pham
Implementation of Genetic Algorithms to Optimize Metal-Organic Frameworks for CO₂ Capture
- 6:30p – 9:30p** **Dinner, Campus Club Lounge Corridor & Terrace, Coffman Memorial Union**
(300 Washington Ave SE, Minneapolis, MN 55455)

Tuesday, April 5, 2022

- 8:00a – 9:00a** **Breakfast**
- 9:00a – 11:00a Working Group on Porting Software to Exascale
Led by Christopher Knight & Alvaro Vazquez-Mayagoitia
- 11:00a – 12:00p** **Boxed Lunch**

April 4 – April 5, 2022 | University of Minnesota

Monday, April 4, 2022

<https://umn.zoom.us/j/94393503092?pwd=aXdzeHFHMHhZNys1R2VaNWNQSGJmdz09>

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Tuesday, April 5, 2022

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NANOPOROUS MATERIALS GENOME CENTER
2022 ALL-HANDS MEETING | ATTENDEE LIST

April 4 – April 5, 2022 | University of Minnesota

EXECUTIVE COMMITTEE

Ilja Siepmann	University of Minnesota	Director Principal Investigator
Donald Truhlar	University of Minnesota	Deputy Director Thrust D Representative* Co-Investigator
Alán Aspuru-Guzik	University of Toronto	Thrust A Representative* Co-Investigator
Coray Colina	University of Florida	Thrust C Representative* Co-Investigator
Randall Snurr	Northwestern University	Thrust B Representative* Co-Investigator

INVESTIGATORS

David Cantu	University of Nevada, Reno	Co-Investigator
Laura Gagliardi	University of Chicago	Co-Investigator
Jason Goodpaster	University of Minnesota	Co-Investigator
Maciej Haranczyk	IMDEA Materials	Co-Investigator
Christopher Knight	Argonne National Laboratory	Co-Investigator
Sapna Sarupria	University of Minnesota	Co-Investigator
David Sholl	Georgia Institute of Technology	Co-Investigator
Alvaro Vazquez-Mayagoitia	Argonne National Laboratory	Co-Investigator
Jingyun Ye	Clarkson University	Co-Investigator

JUNIOR RESEARCHERS

Farideh Badichi Akher	University of Minnesota (Truhlar)	Postdoctoral Associate
Jie Bao	University of Minnesota (Truhlar)	Postdoctoral Associate
Suman Bhaumik	University of Minnesota (Truhlar)	Graduate Student
Saumil Chheda	University of Minnesota (Gagliardi/ Siepmann)	Graduate Student
Brianna Collins	University of Minnesota (Goodpaster)	Graduate Student
Alexander Demidov	University of Florida (Colina)	Graduate Student
Daniel Graham	University of Minnesota (Goodpaster)	Graduate Student
Miguel Hernández del Valle	IMDEA (Haranczyk)	Graduate Student
Andrew Johannesen	University of Minnesota (Goodpaster)	Graduate Student
Siriluk Kanchanakungwankul	University of Minnesota (Truhlar)	Graduate Student
Zhao Li	Northwestern University (Snurr)	Graduate Student
Maryam Mansoori Kermani	University of Minnesota (Truhlar)	Postdoctoral Associate
Abhishek Mitra	University of Chicago (Gagliardi)	Graduate Student
Jiaxin Ning	University of Minnesota (Truhlar)	Graduate Student
Aiswarya M. Parameswaran	University of Minnesota (Truhlar)	Graduate Student
Roshan Ashokbhai Patel	University of Minnesota (Siepmann)	Graduate Student
Thang Pham	Northwestern University (Snurr)	Graduate Student
Jesse Prelesnik	University of Minnesota (Siepmann)	Postdoctoral Associate
Purna	University of Minnesota (Siepmann)	Graduate Student

April 4 – April 5, 2022 | University of Minnesota

JUNIOR RESEARCHERS, CONTINUED....

Kaihang Shi Early Career Network Representative	Northwestern University (Snurr)	Postdoctoral Associate
Richard Shiery	University of Nevada, Reno (Cantu)	Graduate Student
Yangzesheng (Andrew) Sun	University of Minnesota (Siepmann)	Graduate Student
Naomi Trampe	University of Minnesota (Sarupria/Siepmann)	Graduate Student
Dihua Wu	University of Minnesota (Truhlar)	Postdoctoral Associate
Yuhan Yang	Georgia Institute of Technology (Sholl)	Graduate Student
Dayou Zhang	University of Minnesota (Truhlar)	Graduate Student
Jorge Zorrilla Prieto	IMDEA (Haranczyk)	Graduate Student

STAFF

Ethan Ashbrook	University of Minnesota	Scientific Support
Melanie Burns	University of Minnesota	Managing Director
Lisa Zeeb	University of Minnesota	Designer

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

* Thrust B: Development of Exascale Ready Software

* Thrust C: Development of Nanoporous Materials for Challenging Chemical Separations

* Thrust D: Discovery of Porous Materials for Challenging Chemical Transformations

ACKNOWLEDGEMENT

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CHEMICAL SCIENCES PROGRAM.