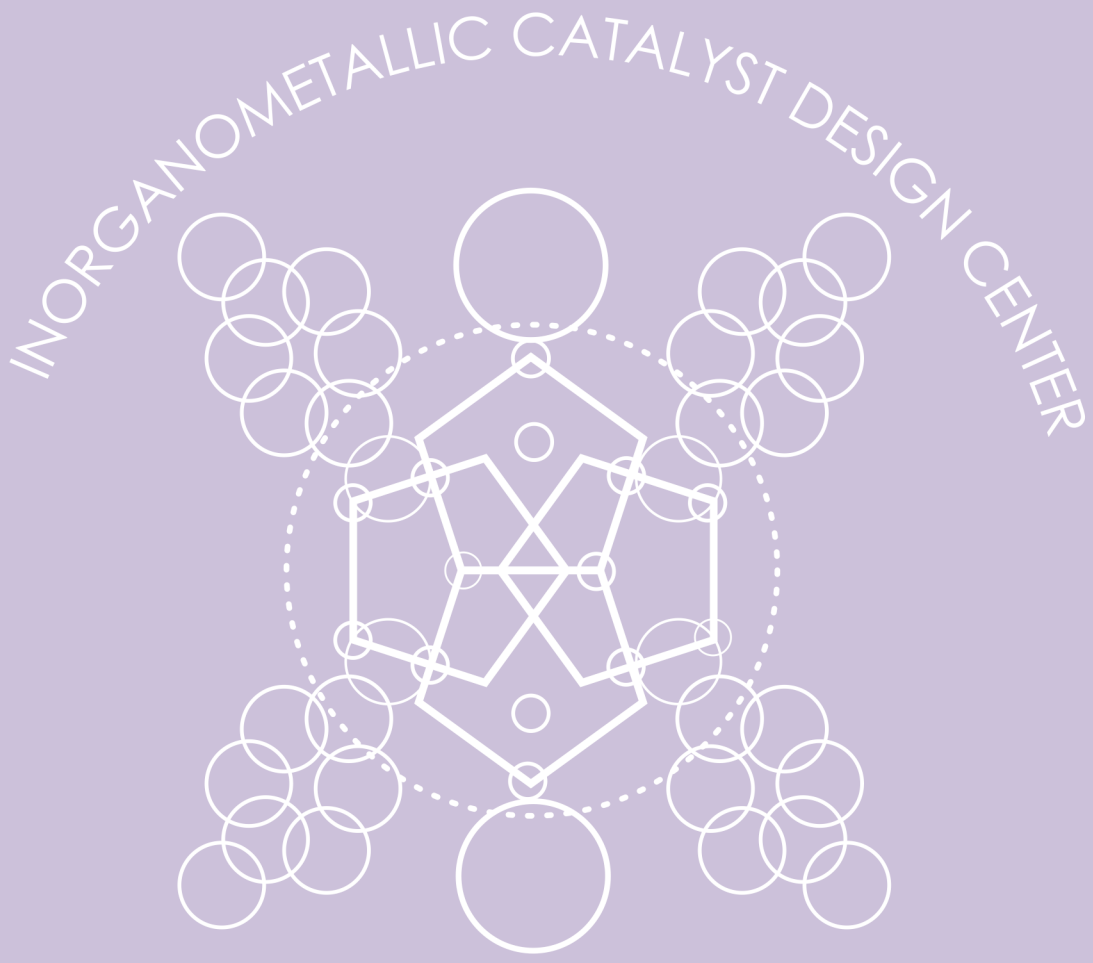

2019 ALL-HANDS MEETING

October 7 – 8, 2019

Argonne NATIONAL LABORATORY

CLEMSON UNIVERSITY

MIT

Northwestern University

NuMat TECHNOLOGIES

Pacific Northwest NATIONAL LABORATORY

Stony Brook University

UCDAVIS

Inorganometallic Catalyst Design Center
2019 ALL-HANDS MEETING PROGRAM

Sunday, October 6, 2019

5:30p **Dinner,** Crooked Pint Ale House, 501 Washington Ave South

7:00p **Social Activity (Ping Pong)**, Hop 21, 501 Washington Ave South

Monday, October 7, 2019

All events held in Thomas Swain Room, unless otherwise noted

8:00a Registration opens, Continental Breakfast available

8:30a Advisory Board Members meet with Director & Deputy Director (Gateway Room)

9:00a **Meeting Begins**
Welcome by Laura Gagliardi

Theme 1 True single-site, MOF- supported catalysts

Topic 1a. Alkane Oxyfunctionalization *(Chair: Jian Liu)*

9:15a Introduction by Omar Farha

9:20a Talk 1 Melike Babucci (University of California, Davis)

"Structure of Fe Sites for Light Alkane Activation Situated in the Nodes of a Metal Organic Framework"

9:30a Talk 2 Matt Simons (University of Minnesota)

"Reactivity of Fe sites for light alkane activation situated in the nodes of a Metal Organic Framework"

9:40a Talk 3 Xuan Zhang (Northwestern University)

"Structure-Activity Relationships and Support Effects in Metal-Organic Frameworks-Supported Vanadium Catalysts"

9:50a Talk 4 Mukunda Mandal (University of Minnesota)

"Computational Characterization of Metal-Organic Frameworks-Supported Vanadium Catalysts for Alcohol Oxidation"

10:00a Talk 5 Carlo Alberto Gaggioli (University of Minnesota)

"Mechanistic Study of *tert*-Butyl Alcohol Dehydration on UiO-66 MOF"

10:10a Summary of Talks 1-5 by Aditya Bhan, Bruce Gates

10:25a Break

Topic 1b. Oligomerization *(Chair: Rebecca Combs)*

10:40a Introduction by Matt Neurock

10:45a Talk 6 Jian Zheng (Pacific Northwest National Laboratory)

"Coordination of Metal Cations at Zr Nodes and Their Catalytic Activity for Dimerization and Oxidation"

10:55a Talk 7 Tim Goetjen (Northwestern University)
"A Cr-Based MOF Supported Heterogeneous Catalyst for Olefin Oligomerization"

11:05a Talk 8 Navneet Khetrapal, Saumil Chheda & Benjamin Yeh (University of Minnesota)
"Mechanistic Insights into Olefin Oligomerization on Transition-Metal Decorated UiO66 MOF"

11:15a Talk 9 Ryan Hackler (Argonne National Laboratory)
"Propyne Oligomerization Catalyzed by Indium-Metallated Metal-Organic Frameworks"

Topic 1c. Aldol Condensation *(Chair: Melike Babucci)*

11:25a Introduction by Johannes Lercher

11:30a Talk 10 Thais Scott (University of Minnesota)
"Aldol Condensation Catalyzed by the Metal Organic Framework UiO-66"

11:40a Summary of Talks 6-10 by Oliver Gutierrez Tinoco, Matt Neurock, Johannes Lercher

12:00p Working Lunch

Topics 1d. Hydrogenation & 1e. Sulfur-containing *(Chair: Carlo Alberto Gaggioli)*

1:05p Introduction by Joe Hupp

1:10p Talk 11 Hafeera Shabbir (Clemson University)
"Elucidation of the Mechanism of Ethylene Hydrogenation on NU-1000 - An Experimental and Microkinetic Study"

1:20p Talk 12 Sai Puneet Desai (University of Minnesota)
"Probing Promoter Effects in Alkyne Semihydrogenation"

1:30p Talk 13 Yifeng Zhu, *presented by Oliver Y. Gutiérrez* (Pacific Northwest National Laboratory)
"Maximizing the Interface Between Zirconia Nodes and Cu Particles for CO_2 Hydrogenation to Methanol"

1:40p Talk 14 Jian Liu (Northwestern University)
"Sulfur-containing and Sulfur-enabled Metal-ion Clusters for MOF-based Heterogeneous Catalysis"

1:50p Summary of Talks 11-14 by Max Delferro

2:05p Break

2:15p Discussion on Theme 1

Theme 2 Advances in synthesis techniques for new MOF-supported catalysts and structural characterization of catalysts *(Chair: Hafeera Shabbir)*

3:00p	Introduction by Lee Penn
3:05p	Talk 15 Rebecca Combs (University of Minnesota)
	"Synthesis of NU-1000: Size and Aspect Ratio"
3:15p	Talk 16 Dan O'Nolan (Stony Brook University)
	"*In-situ* Total Scattering Studies: New Tools and Techniques for MOF-Catalyst Characterization"
3:25p	Talk 17 Zoha Syed (Northwestern University / Argonne National Laboratory)
	"Mechanistic Insights into C-H Borylation with MOF-supported (Phen)Ir Complexes"
3:35p	Summary of Talks 15-17 by Karena Chapman
3:45p	Break

Theme 3 Advances in theoretical/computational methods and data driven discovery *(Chair: Zoha Syed)*

4:00p	Introduction by Rachel Getman
4:05p	Talk 18 Aditya Nandy (Massachusetts Institute of Technology)
	"Machine Learning Approaches for Multi-Objective Catalyst Design"
4:15p	Talk 19 Xin-Ping Wu & Bo Yang (University of Minnesota)
	"Developing QM/MM Methods for Metal-Organic Frameworks and Applying Them for Interpreting Catalytic Experiments"
4:25p	Talk 20 Jingyun Ye (University of Minnesota)
	"Cu Cluster Supported on Defected UiO-66 for CO_2 Hydrogenation to Produce Methanol: What is the Active Site?"
4:35p	Summary of Talks 18-20 by Heather Kulik
4:50p	Break
5:00p	Discussion on Themes 2 and 3
5:30p	Collaboration time
5:30p	Advisory Board Members meet (Gateway Room)
6:00p	**Appetizers and Drinks available (Heritage Gallery)**
6:30p	**Dinner (Heritage Gallery)**
7:30p	**Public Lecture "Model Systems for Heterogeneous Catalysts at the Atomic Level"**
	Hans-Joachim Freund, Fritz-Haber-Institut der Max-Planck-Gesellschaft

Tuesday, October 8, 2019

All events held in Thomas Swain Room, unless otherwise noted

8:00a	Continental Breakfast available
8:30a	Advisory Board Members meet with Director and Deputy Director (Gateway Room)
9:00a	**Group Discussion: Current and future priorities** *Moderated by Laura Gagliardi and Joe Hupp*
10:00a	**Group Photo**
10:15a	**Group Discussion: How to prepare for the mid-term review & Collaboration time**
11:15a	Break
11:30a	Buffet Lunch

DOE Chris Bradley site visit

1:00p	**Welcome by Chris Cramer, Vice President for Research**
1:15p	**Short Research Summary Talks**
	1:15p Laura Gagliardi
	1:30p Joe Hupp
	1:45p Aditya Bhan
	2:00p Karena Chapman
2:15p	**Discussion**
2:30p	**Poster session, with refreshments**
4:30p	UMN Chemistry Lab Tours (Smith Hall)
5:30p	Debrief with Chris Bradley and Center Management (Smith Hall, 101J)
6:30p	Dinner, Haiku Japanese Bistro, 620 Washington Ave SE, Minneapolis, MN 55414

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.

No.	Title	First / Joint Co-Author(s)
01	Activating MOF Catalysts: Time, Temperature and Atmosphere-Based Research	Zhihengyu Chen (Stony Brook)
02	Tests of Local Functionals for Predicting Condensed-Phase Structural and Electronic Properties, Including Nanoporous Materials	Indrani Choudhuri (UMN)
03	Synthesis of NU-1000: Size and Aspect Ratio	Rebecca Combs (UMN)
04	Multiconfigurational Calculations on Bimetallic Decorated NU-1000 for C–H Activation and Comparison with DFT	Carlo Alberto Gaggioli (UMN)
05	A Cr-Based MOF Supported Heterogeneous Catalyst for Olefin Oligomerization	Tim Goetjen (Northwestern)
06	Propyne Oligomerization Catalyzed by Indium-Metallated Metal-Organic Frameworks	Ryan Hackler (ANL)
07	Mechanistic Insights into Olefin Oligomerization on Transition-Metal Decorated UiO66 MOF	Navneet Khetrapal & Saumil Chheda (UMN)
08	Computational Investigation of Ligand-Modulated Ethylene Hydrogenation on NU-1000	Daniel King (UMN)
09	Sulfur-containing and Sulfur-enabled Metal-ion Clusters for MOF-based Heterogeneous Catalysis	Jian Liu, Qin Liu & Qining Wang (Northwestern)
10	Accelerating Catalyst Discovery with Machine Learning and Automation	Aditya Nandy & Michael Taylor (MIT)
11	*In-situ* Total Scattering Studies: New Tools and Techniques for MOF-Catalyst Characterization	Daniel O'Nolan (Stony Brook)
12	Computational Studies of Isomerization and Selective Hydrogenation of Propyne on Metal Clusters Deposited on NU-1000	Riddhish Pandharkar (UMN)
13	Oxidation of Strong C-H Bonds Using Metal Organic Frameworks	Steven Prinslow & Sai Puneet Desai (UMN)
14	Aldol Condensation Catalyzed by the Metal Organic Framework UiO-66	Thais Scott (UMN)
15	Elucidation of the Mechanism of Ethylene Hydrogenation on NU-1000 - An Experimental and Microkinetic Study	Hafeera Shabbir (Clemson)
16	Structure, Dynamics, and Reactivity of Fe(II) Sites Situated in the Nodes of a Metal-Organic Framework for Light Alkane Oxidation	Matt Simons (UMN) & Melike Babucci (UC Davis)
17	Mechanistic Insights into C-H Borylation with MOF-supported (Phen)Ir Complexes	Zoha Syed (Northwestern / ANL)
18	MOF-templated Au-Cu Bimetallic Nanoparticle Catalysts for CO Oxidation	Mark Taylor (Northwestern)
19	Periodic or Cluster Model?: Benchmarking Metal-Organic Framework Models	Stephen Vicchio (Clemson)
20	Developing QM/MM Methods for Metal-Organic Frameworks and Applying Them for Interpreting Catalytic Experiments	Xin-Ping Wu & Bo Yang (UMN)
21	Selective Oxidation of Alkanes by Copper-oxo Species Supported on Metal−Organic Frameworks	Ying Yang (Northwestern)
22	Propylene Oligomerization on Nickel UiO-66 MOF	Benjamin Yeh (UMN)
23	Structure-Activity Relationships and Support Effects in Metal-Organic Frameworks-Supported Vanadium Catalysts	Xuan Zhang (Northwestern)
24	Coordination of Metal Cations at Zr Nodes and Their Catalytic Activity for Dimerization and Oxidation	Jian Zheng (PNNL)

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