



**ICDC All-Hands Meeting**  
**The Saint Paul Hotel, Promenade Ballrooms and Foyer**  
**Agenda**  
**Monday, September 11, 2017**

7:30 am	<b>Registration</b> Continental Breakfast Available	Prom Foyer	All
8:30 am	<b>Director's Welcome</b>	Prom South	Laura Gagliardi
<b>THEME 1: CATALYSIS</b> <b>(Chair: Joe Hupp)</b>			
8:40 am	<b>Presentation #1</b>	Prom South	
	Ethanol Dehydration Catalyzed by Zr <sub>6</sub> O <sub>8</sub> Nodes in Metal–Organic Frameworks: Probing the Structure and Dynamics of Node Surfaces in UiO-66, UiO-67, and NU-1000		Dong Yang, Manuel A. Ortuño, Varinia Bernales, Christopher J. Cramer, Laura Gagliardi, and Bruce C. Gates
8:55 am	<i>Discussion</i>		
9:05 am	<b>Presentation #2</b>	Prom South	
	Pt clusters and nanoparticles deposited on the nodes of NU-1000 for ethylene hydrogenation		Jian Zheng, Andreas Mavrantoukakis, Steven L. Pellizzeri, Zhanyong Li, Rachel B. Getman, John L. Fulton, Oliver Y. Gutiérrez, Donald M. Camaioni, Christopher J. Cramer, Laura Gagliardi, Omar K. Farha, Joseph T. Hupp, and Johannes A. Lercher
9:20 am	<i>Discussion</i>		
9:30 am	<b>Presentation #3</b>	Prom South	
	Computational Study of MOF-Supported Transition Metal Catalysts for Ethylene Dimerization		Jingyun Ye, 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
9:45 am	<i>Discussion</i>		
9:55 am	<b>Presentation #4</b>	Prom South	
	Screening Supported Nanocatalysts for Ethene Conversions		Steven Pellizzeri, Pere Miro, Varinia Bernales, Melissa Barona, In Soo Kim, Peilin Liao, Alex Martinson, Laura Gagliardi, Randall Snurr, and Rachel Getman
10:10 am	<i>Discussion</i>		
10:20 am	<b>BREAK</b>	Prom Foyer	All
10:50 am	<b>Presentation #5</b>	Prom South	
	Fine-Tuning the Activity of Metal–Organic Framework-Supported Cobalt Catalysts for the Oxidative Dehydrogenation of Propane		Zhanyong Li, Matt Simons, Aaron W. Peters, Ana E. Platero-Prats, Varinia Bernales, Manuel A. Ortuño, Karena W. Chapman, Neil M. Schweitzer, Jian Liu, Chung-Wei Kung, Matthew R. DeStefano, Hyunho Noh, Christopher J. Cramer, Laura Gagliardi, Joseph T. Hupp, and Omar K. Farha
11:05 am	<i>Discussion</i>		

<b>11:15 am</b>	<b>Presentation #6</b>	Prom South	
	Semi-hydrogenation of alkynes using a MOF based heterobimetallic catalyst		Sai Puneet Desai, Jingyun Ye, Jian Zheng, Camille D. Malonzo, Thomas Webber, Leighanne C. Gallington, Matthew R. DeStefano, Omar K. Farha, Joseph T. Hupp, Karena W. Chapman, Laura Gagliardi, R. Lee Penn, Andreas Stein John Fulton, Donald Camaioni, and Connie C. Lu
11:30 am	<i>Discussion</i>		
<b>11:40 am</b>	<b>Presentation #7</b>	Prom South	
	Pushing the limits on NU-1000 as a catalyst support		Sol Ahn, Emily Cheng, Laruen McCullough, Omar Farha, Justin Notestein
11:55 am to 12:05 pm	<i>Discussion</i>		
<b>12:30 pm</b>	<b>BUFFET LUNCH</b>	Prom North	All
<b>THEME 2: NOVEL MATERIALS AND MATERIAL CHARACTERIZATION (Chair: Alex Martinson)</b>			
<b>2:00 pm</b>	<b>Presentation #8</b>	Prom South	
	Localizing catalyst-substrate interactions in NU-1000 catalysts	Prom South	Ana E. Platero-Prats, Jian Liu, Zhanyong Li, Leighanne C. Gallington, Joseph T. Hupp, Omar K. Farha, Karena W. Chapman
2:15 pm	<i>Discussion</i>		
<b>2:25 pm</b>	<b>Presentation #9</b>	Prom South	
	Towards Single-Site Catalysts: Achieving a Simpler Node Structure in NU-1000 via Active Site Blocking Approach		In Soo Kim, Nicolaas A. Vermeulen, Omar K. Farha, Joseph T. Hupp, Alex B. F. Martinson
2:40 pm	<i>Discussion</i>		
<b>2:50 pm</b>	<b>Presentation #10</b>	Prom South	
	Extending the Scope of Nanocasting in Metal–Organic Frameworks		Wenyang Zhao, Zhao Wang, Camille Malonzo, Jiaxin Duan, Thomas Webber, Ana E. Platero-Prats, Francisco Sotomayor, Zhanyong Li, In Soo Kim, Omar Farha, Joseph Hupp, Alex Martinson, Karena W. Chapman, Matthias Thommes, R. Lee Penn, <u>Andreas Stein</u>
3:05 pm	<i>Discussion</i>		
<b>3:15 pm</b>	<b>Presentation #11</b>	Prom South	
	Non-Innocent Catecholate Ligand on the Activity of Metal–Organic Frameworks-Supported Cu Catalysts		Xuan Zhang, Nicolaas A. Vermeulen, Zhiyuan Huang, Yuexing Cui, Jian Liu, Matthew D. Krzyaniak, Zhanyong Li, Hyuno Noh, Michael R. Wasielewski, Massimiliano Delferro, and Omar K. Farha
3:30 pm	<i>Discussion</i>		
<b>3:40 pm</b>	<b>BREAK</b>	Prom Foyer	All
<b>3:40 pm</b>	<b>POSTER SETUP</b>	Prom North	All poster presenters may start setting up during the break. All posters to be set up by the start of the poster session.

**THEME 3: THEORETICAL ADVANCES**  
**(Chair: Chris Cramer)**

<b>4:00 pm</b>	<b>Presentation #12</b>	Prom South	
	Combined Quantum Mechanical and Molecular Mechanical Method for Catalyst Design on the NU-1000 Metal-Organic Framework		<u>Xin-Ping Wu</u> , Laura Gagliardi and Donald G. Truhlar
<i>4:15 pm</i>	<i>Discussion</i>		
<b>4:25 pm</b>	<b>Presentation #13</b>	Prom South	
	Computational Screening and Predictive Catalyst Design of Metal-Organic Frameworks for the Oxidation of Methane and Ethane		<u>Andrew S. Rosen</u> , Peilin Liao, Hieu A. Doan, Melissa Barona, Rachel B. Getman, Randall Q. Snurr
<i>4:40 pm</i>	<i>Discussion</i>		
<b>4:50 pm</b>	<b>Presentation #14</b>	Prom South	
	Inorganometallic Catalyst Design: Alkane Metathesis Catalysis in NU-1000 MOFs Functionalized with Transition Metals		<u>Bo Yang</u> , Kamal Sharkas, Laura Gagliardi, and Donald G. Truhlar
<i>5:05 pm</i>	<i>Discussion</i>		
<b>5:15 pm</b>	<b>Presentation #15</b>	Prom South	
<b>5:15 pm</b>	Quantum Monte Carlo Calculations of Energy Barrier Heights		Anouar Benali, Hyeondeok Shin, Aaron League, Dale Pahls, Jingyun Ye, Chris Cramer, Laura Gagliardi, and <u>Olle Heinonen</u>
<i>5:30 pm</i>	<i>Discussion</i>		
<b>5:40 pm</b>	<b>END TALKS</b>		
<b>6:30 pm</b>	<b>BUFFET DINNER</b>	Prom South	All
<b>8:00 pm to 9:30 pm</b>	<b>POSTER SESSION and DESSERT</b>	Prom North	All
<b>9:30 pm</b>	<b>POSTER REMOVAL</b>	Prom North	All posters must be removed and out of the room immediately following the end of the poster session.
<b>9:30 pm</b>	<b>Meeting Ends</b>		