



## Abstract Roster and Poster List

**Poster Session**  
**Saint Paul Hotel, Promenade Ballroom North**  
**8:00 pm - 9:30 pm**  
**Monday, September 11, 2017**

NOTE: This is a list of all the abstracts received, in alphabetical order by first author(s). Not all abstracts submitted resulted in a poster request. If you *are* presenting a poster, please display it on the board tagged with your Poster/Abstract No. If you *are not* presenting a poster, just leave the poster board blank. Do not re-arrange the numbered tags.

Poster/ Abstract No.	Title	First/Joint Co- Author(s)
01	Catalytic Activity of Porphyrin-Supported Iron Oxide Clusters for Methane Oxidation	Barona (NW)
02	A Computational Investigation of Ethylene Dimerization and Hydrogenation Mechanisms on Iridium Deposited NU-1000 and UiO-66	Demir (UMN)
03	Semi-hydrogenation of alkynes using a MOF based heterobimetallic catalyst	Desai (UMN)
04	Deposition of Organometallic Tungsten Precursors on NU-1000 for Alkane Metathesis	Dunn (UMN)
05	Multireference calculations on bimetallic decorated NU-1000 for C–H activation: comparison with DFT	Gaggioli (UMN)
06	Development of Heterobimetallic Precursors toward Preparation of Lewis Acid-Modified Group 10 Single Sites on NU-1000	Garr (UMN)
07	Quantum Monte Carlo Calculations of Energy Barrier Heights	Heinonen (ANL)
08	Theoretical Insights into Selective Oxidation of Methane to Methanol on Porphyrin-supported Copper Oxide Nanoclusters	Doan (NW)
09	Towards Single-Site Catalysts: Achieving a Simpler Node Structure in NU-1000 via Active Site Blocking Approach	Kim (ANL)
10	Fine Tuning the Activity of Metal–Organic Framework-Supported Cobalt Catalysts for the Oxidative Dehydrogenation of Propane	Li (NW)
11	Tuning Catalytic Reactivity and Selectivity of MOF-Supported Nickel through Electronic Effect of Modified Ligands	Liu (NW)
12	Hydrolysis of Chemical Warfare Agents on Metal Organic Frameworks	Momeni (UMN)
13	Pushing the limits on NU-1000 as a catalyst support	Notestein (NW)

Poster/ Abstract No.	Title	First/Joint Co- Author(s)
14	Screening Supported Nanocatalysts for Ethene Conversions	Pellizzeri (Clemson)
15	Localizing catalyst-substrate interactions in NU-1000 catalysts	Platero-Prats (ANL)
16	Computational Screening and Predictive Catalyst Design of Metal-Organic Frameworks for the Oxidation of Methane and Ethane	Rosen (NW)
17	Correlated-Participating-Orbitals Pair-Density Functional Method for Calculating the Bond Dissociation energies of FeX and NiX (X= C, S, Se)	Sharkas (UMN)
18	C–H Bond activation on bimetallic two-cation Co-M oxide clusters deposited on Zr-based MOF nodes: Effects of doping at the molecular level	Simons (UMN)
19	Extending the Scope of Nanocasting in Metal–Organic Frameworks	Stein (UMN)
20	Immobilization of Earth Abundant Metals Coordinated in Heterobimetallic Ligand Scaffolds on Metal Organic Frameworks (MOFs)	Vitillo (UMN)
21	Carbon Nanocasting in NU-1000	Wang (UMN)
22	Role of Modulator in the Synthesis of Phase-Pure NU-1000	Webber (UMN)
23	Combined Quantum Mechanical and Molecular Mechanical Method for Catalyst Design on the NU-1000 Metal-Organic Framework	Wu (UMN)
24	Inorganometallic Catalyst Design: Alkane Metathesis Catalysis in NU-1000 MOFs Functionalized with Transition Metals	Yang, B. (UMN)
25	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	Yang, D. (UC Davis) and Ortuño, M. (UMN)
26	Computational Study of MOF-Supported Transition Metal Catalysts for Ethylene Dimerization	Ye (UMN)
27	Non-Innocent Catecholate Ligand on the Activity of Metal-Organic Frameworks-Supported Cu Catalysts	Zhang (NW)
28	Synthesis of TiO <sub>2</sub> -stabilized Oxozirconium Clusters through Nanocasting in NU-1000	Zhao (UMN)
29	Pt clusters and nanoparticles deposited on the nodes of NU-1000 for ethylene hydrogenation	Zheng (PNNL), Mavrantakis (UMN), Pellizzeri (Clemson)
30	Ion-exchanged Cu-NU-1000 for selective methane oxidation	Zheng (PNNL), Ortuño (UMN)