



Abstract Roster and Poster List

Poster Session, Promenade Ballroom North
 8:00 pm - 9:30 pm
 Monday, August 15, 2016

Pres. No.	Poster No.	Title	First/Joint Co-Author(s)/Presenter
N/A	01	Parallel CASSCF Calculations Beyond the Limits of the Conventional CASSCF Implementations	Vogiatzis (UMN)
N/A	02	Synthesis of TiO ₂ -stabilized Single-site Oxozirconium Clusters through Nanocasting in NU-1000	Zhao (UMN)
N/A	03	Nanocasting NU-1000 with Carbon	Wang (UMN)
10	04	Thermal Stabilization of Metal-Organic Framework-Derived Catalytic Single Sites Through Nanocasting	Malonzo (UMN)
N/A	05	Multiconfiguration Pair-Density Functional Theory: Recent Developments for Ground and Excited-State Chemistry	Carlson (UMN)
N/A	06	Probing the Catalytic Activity of Bimetallic-Functionalized Metal Organic Frameworks	Desai (UMN) and Moore (UMN)
N/A	07	Catechol-Ligated Transition Metals: A Quantum Chemical Study on a Promising System for Gas Separation	Stoneburner (UMN)
3	08	Oxidative Dehydrogenation of Propane Catalyzed by Co-decorated NU-1000	Li, Zhanyong (NW) and Ortuño (UMN)
2	09	Cu-NU-1000: Structural Characterization and Catalytic Activity for Methane Oxidation	Zheng (PNNL) and Ortuño (UMN)
1	10	Tuning the Sites on Metal Oxide-Like MOF Clusters as Supports for Well-Defined Metal Complex Catalysts	Yang (UC Davis) and Bernales (UMN)
N/A	11	NU-1000 Supported Niobium Catalysts: In-situ Active Sites Titration & Cyclohexene Epoxidation	Ahn (NW)
5	N/A	Extending scaling relationships from unsupported to supported metal cluster catalysts	Pellizzeri (Clemson)
N/A	12	Exploring Catalysis Opportunities of Iridium Deposited NU-1000 and UiO-66	Demir (UMN)
N/A	13	Catalytic Activity of Porphyrin-Supported Mixed Metal Oxide Nanoclusters	Barona (NW)
6	N/A	Hydrogenation and Oligomerization of Ethylene Catalyzed by Transition Metal Oxide Nanoclusters	Barona (NW) and Pellizzeri (Clemson)
N/A	14	Testing a Simple Gaussian Model for Vibronic Band Shapes in Electronic Spectroscopy	Li, Shaohong (UMN)
N/A	15	Alkane Metathesis Catalysis in Ta/W-Functionalized NU-1000 MOFs	Yang, Bo (UMN)
7	N/A	Evolution of metal distribution in metal-organic frameworks during atomic layer deposition: Single-site catalyst deposition in NU-1000 is directed to small pores by dispersion interactions	Gallington (ANL) and Liu (UMN)

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8	N/A	Platinum Atomic Layer Deposition (ALD) in Metal-Organic Framework (MOF) for Ethylene Hydrogenation	Kim (ANL), Li, Zhanyong (NW), Zheng (PNNL), and Mavrantonas (UMN)
N/A	16	Diversifying and Understanding Atomic Layer Deposition (ALD) in Metal-Organic Frameworks (MOF) for High-Throughput Catalysis Testing	Kim (ANL)
N/A	17	Computational investigation of ethylene hydrogenation with small metal clusters deposited on NU-1000	Mavrantonas (UMN)
N/A	18	Adsorption of ethylene by the mesoporous catalyst Ni-NU-1000	Gallington (ANL)
N/A	19	The nature and structure of Pt-NU-1000 for ethylene hydrogenation: an in situ XAFS and DFT study	Zheng (PNNL) and Mavrantonas (UMN)
4	N/A	Deposition and Activity of Heterobimetallic Complexes onto NU-1000	Desai (UMN) and Pahls (UMN)
9	20	Size and Phase Control of a Metal-Organic Framework	Webber (UMN)
N/A	21	Metal exchange in the zirconia node of NU-1000 for catalysis	Pham (UMN)
N/A	22	Correlation and Holes: Visualizing Electron Correlation as a Function of Active Space	Sharma (UMN)
12	N/A	Catalytic Behavior of Few-atom Metal Sulfide Clusters Deposited Within the Metal-Organic Framework NU-1000	Peters (NW)
11	23	DFT Study of MOF-Node as Support for Tungsten Metathesis Catalyst	Qu (UMN)
4:40 pm	N/A	Towards an Understanding of Supported Metal Oxides and Sulfides for Chemicals Synthesis	Notestein (NW)
4:55 pm	N/A	Mechanistic studies of heterogeneous catalytic systems: A case study on partial oxidation of light olefins	Bhan (UMN)
5:10 pm	N/A	New applications of early transition metals in catalysis	Tonks (UMN)
POSTER-ONLY ADDITIONS, Post-Published List			
N/A	24	Multiconfiguration Pair-Density Functional Theory: Affordability and Accuracy in Multireference Calculations	Sand (UMN)
N/A	25	Ir Complexes Deposited on Al(III) Decorated Nu-1000: A Highly Selective Catalyst for Ethylene Hydrogenation and Dimerization	Momeni (UMN)
N/A	26	Reaching consensus on the structural nature of the nickel sites within NU-1000	Platero-Prats (ANL)