

**AGENDA**  
**New England Catalysis Society Winter Meeting**

8:50-9:00	<i>Welcome and Introductory remarks</i>
9:00 – 10:00	<p><b>Plenary Lecture: Operando Methods for the Characterization of Energy Materials</b>  <i>Prof. Héctor D. Abruña</i>  <i>Department of Chemistry &amp; Chemical Biology and Energy Materials Center Cornell University</i></p>
10:00-10:20	<p><b>Controlling Hydrogen Dissociation, Spillover and Storage using the Molecular Cork Effect</b>  <i>Matthew D. Marcinkowski<sup>1</sup>, April D. Jewell<sup>1</sup>, Michail Stamatakis<sup>2</sup>, Matthew B. Boucher<sup>3</sup>, Emily A. Lewis<sup>1</sup>, Colin J. Murphy<sup>1</sup>, Georgios Kyriakou<sup>1</sup> and E. Charles H. Sykes<sup>1</sup></i>  <sup>1</sup> Tufts University Chemistry<sup>2</sup> University College London Chemical Engineering, <sup>3</sup> Tufts University Chemical Engineering</p>
10:20-10:40	<p><b>Dominance of Surface Pore Blockages in Hierarchical Zeolites</b>  <i>Andrew R Teixeira,</i>  <i>Massachusetts Institute of Technology, Department of Chemical Engineering,</i>  <i>77 Massachusetts Ave., Cambridge, MA 02139. <a href="mailto:ateix@mit.edu">ateix@mit.edu</a></i></p>
10:40-11:00	Coffee Break – Membership Fee Collection
11:00-11:20	<p><b>Catalytic Conversion of CO<sub>2</sub> Greenhouse Gas into Value-added Products</b>  <i>Boxun Hu<sup>1#</sup>, Steven L. Suib<sup>1, 2</sup></i>  <i>Institute of Materials Science, 97 North Eagleville Road, University of Connecticut</i></p>
11:20-11:40	<p><b>Understanding the Activity of Nanoporous Gold Catalysts for Sustainable Oxidation Reactions</b>  <i>Branko Zujic, Michelle Personick, Lucun Wang, Kara Stowers, Robert J Madix, Cynthia M Friend</i>  <i>Department of Chemistry, Harvard University</i></p>
11:40-12:00	<p><b>Methane to Acetic Acid over Cu-exchanged Zeolites: Mechanistic Insights from a Site Specific Carbonylation Reaction</b>  <i>Karthik Narsimhan, Vladimir K. Michaelis, Guinevere Mathies, William R. Gunther, Robert G. Griffin, and Yuriy Román-Leshkov</i>  <i>Massachusetts Institute of Technology</i></p>
12:00-12:20	<p><b>Manganese Oxide Nanoparticles with High Overpotential for Hydrogen and Oxygen Evolution: Breaking Potential Window Limit of Aqueous Electrochemical Energy Storage</b>  <i>Xiaowei Teng<sup>1*</sup>, Xiaoqiang Shan<sup>1</sup>, Daniel S. Charles<sup>1</sup>, Guofeng Wang<sup>2</sup>, Mikhail Feygenson<sup>3</sup></i>  <sup>1</sup>Department of Chemical Engineering, University of New Hampshire <sup>2</sup></p>

	<i>Department of Chemical Engineering, University of Pittsburgh  <sup>3</sup>Spallation Neutron Source, Oak Ridge National Laboratory</i>
12:20-1:30	LUNCH
1:30-2:10	<b>Keynote Lecture: Teaching Sponges New Tricks: Redox Reactivity in Microporous Metal-Organic Frameworks</b> <i>Prof. Mircea Dincă Department of Chemistry  Massachusetts Institute of Technology</i>
2:10-2:30	<b>Design of Lattice Strain in Shaped Pd-Ni-Pt Core-Sandwich-Shell Nanoparticles: Influence of Ni Sandwich Layers on Catalytic Electrooxidations for Fuel Cells</b> <i>Brian T. Sneed †, Allison P. Young †, Daniel Jalalpoor ‡, Matthew C. Golden †, Shunjia Mao †, Ying Jiang §, Yong Wang §, and Chia-Kuang Tsung †*</i> † <i>Department of Chemistry, Merkert Chemistry Center, Boston College, 2609 Beacon Street, Chestnut Hill, Massachusetts 02467, United States</i> ‡ <i>Department of Chemistry, Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin, Germany</i> § <i>Center of Electron Microscopy and State Key Laboratory of Silicon Materials, Department of Materials Science and Engineering, Zhejiang University, Hangzhou 310027, China</i>
2:30-2:50	<b>Metaphosphate chemistry for cathode materials</b> <i>Yanfeng Jiang and Christopher Cummins  Department of Chemistry, Massachusetts Institute of Technology</i>
2:50-3:00	<b>Coffee Break</b>
3:00-3:20	<b>Catalysis on a single nanoparticle using field emission techniques</b> <i>Cédric BARROO  School of Engineering and Applied Sciences, Harvard University</i>
3:20-3:40	<b>Hf-Beta as an Effective Solid Lewis Acid Catalyst for the Coupled Transfer Hydrogenation and Etherification of HMF with Alcohols</b> <i>Jennifer D. Lewis<sup>1</sup>, Stijn Van de Vyver<sup>1</sup>, Anthony J. Crisci<sup>1</sup>, William R. Gunther<sup>1</sup>, Vladimir K. Michaelis<sup>1</sup>, Robert. G. Griffin<sup>1</sup>, and Yuriy Román-Leshkov<sup>1*</sup></i> <sup>1</sup> <i>Massachusetts Institute of Technology</i>
3:40-4:00	<b>Efficient mechano-catalytic depolymerization of crystalline cellulose by formation of branched glucan chains</b> <i>Paul Dornath<sup>1</sup>, Hong Je Cho<sup>1</sup>, Alex Paulsen<sup>2</sup>, Paul Dauenhauer<sup>2</sup> and Wei Fan<sup>1</sup></i> <sup>1</sup> <i>Department of Chemical Engineering, University of Massachusetts</i>

	<p>Amherst, 159 Goessmann Lab, 686 N. Pleasant St., Amherst, MA 01003, USA.</p> <p>2. Department of Chemical Engineering and Materials Science, University of Minnesota, 445 Amundson Hall, 421 Washington Ave SE, Minneapolis, MN 55455, USA.</p>
4:00-5:30	<b>POSTER SESSION IN R&amp;D Commons 4<sup>th</sup> Floor Building 32 – State Center</b>

## Poster Session

#1	<p><b>Imparting Functionality to Biocatalysts via Embedding Enzymes into Nanoporous Materials by a de novo Approach: Size-Selective Sheltering of Catalase in Metal-Organic Framework Microcrystals</b></p> <p>Shao-Chun Wang<sup>†, ‡</sup>, Chia-Kuang (Frank) Tsung<sup>‡</sup></p> <p><sup>†</sup> Department of Chemistry, National Central University, 300 Jhong-Da Road, Chung-Li 32001, Taiwan</p> <p><sup>‡</sup> Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill, Massachusetts 02467, USA</p>
#2	<p><b>The Role of Rhodium on the Electro-oxidation of Ethanol to CO<sub>2</sub></b></p> <p>Guangxing Yang, Xiaowei Teng</p> <p><sup>1</sup>Department of Chemical Engineering, University of New Hampshire</p>
#3	<p><b>PtCu Alloys at the Single Atom Limit for Pt Catalyze Selective Hydrogenation of Butadiene</b></p> <p>Felicia R. Lucci, Jilei Liu, Maria Flytzani-Stephanopoulos and E. Charles H. Sykes</p> <p>Tufts University Chemistry</p>
#4	<p><b>Modeling Iridium-based alloys for ethanol oxidation in fuel cell applications</b></p> <p>Lida Namin and Aaron Deskins</p> <p>Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, Massachusetts</p>
#5	<p><b>Multi-Metallic Nanoparticles: Strain effect on Oxidation Reactions for Applications in Fuel Cell Technologies</b></p> <p>Allison P. Young, Brian T. Sneed, Matthew C. Golden, Daniel Jalalpoor, Chia-Kuang Tsung</p> <p>Department of Chemistry, Merkert Chemistry Center, Boston College</p>
#6	<p><b>Low-Temperature Catalytic Conversion of Ethanol on Au/ZnZrO<sub>x</sub> Nanostructures</b></p> <p>Chongyang Wang<sup>a</sup>, Gabriella Garbarino<sup>b</sup>, Faith Wilson<sup>a</sup>, Guido Busca<sup>b</sup>, Maria Flytzani-Stephanopoulos<sup>a</sup></p> <p><sup>a</sup>Tufts University, Department of Chemical and Biological Engineering, 4</p>

	<p>Colby Street, Medford, MA 02155, USA  <i><sup>b</sup>Università degli Studi di Genova, Dipartimento di Ingegneria Civile, Chimica e Ambientale (DICCA), Laboratorio di chimica delle superfici e catalisi, P.zzale Kennedy, 116129 Genova, Italy</i></p>
#7	<p><b>Gas and Solvent phase Stability of Intermediates in Ethanol oxidation reaction on Pd(111) catalysts – A first principles approach</b>  <i>Satish Kumar Iyemperumal and N. Aaron Deskins</i>  <i>Department of Chemical Engineering, Worcester Polytechnic Institute, Worcester, Massachusetts</i></p>
#8	<p><b>Competition between CO<sub>2</sub> reduction and H<sub>2</sub> evolution on transition metal electrodes</b>  Yin-Jia Zhang and Andrew Peterson  Department of Chemical Engineering, Brown University</p>
#9	<p><b>Engineering Core-Shell Nanocrystal@MOF Nanostructures for Applications: Surfactant-Directed Atomic to Mesoscale Alignment and Capping-Agent-Free Nanoparticles Encapsulation"</b>  <u>Lien-Yang Chou</u>, Pan Hu, Allison P. Young, and Prof. Chia-Kuang (Frank) Tsung  Department of Chemistry, Merkert Chemistry Center, Boston College, Chestnut Hill, Massachusetts 02467, USA</p>
#10	<p><b>Surface Reactions in Lithium Battery Electrodes: Understanding Solid-Electrolyte Interphase Formation with Electronic Structure Calculations</b>  M. A. Gialampouki, A. A. Peterson  <i>School of Engineering, Brown University, Providence, RI 02912, USA</i></p>