# Catalysis Club of Philadelphia

**Thursday February 19th, 2015**
DoubleTree Hotel
4727 Concord Pike Wilmington, DE 19803

**Bridging Heterogeneous Catalysis and Electro-catalysis: Catalytic Reactions Involving Oxygen**

Dr. Umit S. Ozkan

*Department of Chemical and Biomolecular Engineering, The Ohio State University, Columbus, OH*

**&**

**Methane Conversion to Methanol on Copper Containing Small Pore Zeolites**

**Bahar Ipek**, Matthew J. Wulfers, Shewangizaw Teketel, Raul F. Lobo

*Department of Chemical and Biomolecular Engineering University of Delaware, Wilmington, DE*

**Social Hour:** **5:30 PM**
**Dinner:** **6:30 PM**
**Meeting:** **7:30 PM**

**Members:** $35.00
**Walk Ins & Non-members:** $40.00
**Student & Retired Members:** $20.00

## *Menu*

**Roasted Pork** – fennel, orange, crushed red pepper served with parmesan polenta and Brussels with pancetta

**Salmon Romanesco** – salmon with romesco sauce served with creamy polenta and broccoli rabe

**Veg Filo Triangle** – roasted vegetables wrapped in filo dough

**Meal reservations** - Please notify your company representative or Eyas Mahmoud (eyas@udel.edu) by ***Thursday February 12th*** , or register online: http://catalysisclubphilly.org/ program/ meeting-registration/

Company Representatives – We would like to encourage you to make meal/meeting reservations to your company representative.

**Membership** - Dues for the 2014-15 season will be $25.00 ($5.00 for the local chapter and $20.00 for the national club). Dues for students, post-docs and retirees will be $10.00 ($5.00 for local club and $5.00 for national club).

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**Catalytic Reactions Involving Oxygen**

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*The Ohio State University*

**Abstract**. Catalytic reactions that involve oxygen can be found in a large number of processes, including those in energy-related applications, in emission control and in processes important for the chemical industry. Whether the catalytic reaction is an oxygen insertion step as in a selective oxidation reaction, or an oxygen removal step as in a hydrodeoxygenation reaction, oxygen has proven to be a very challenging component, often determining the selectivity of the reaction. Some examples from our laboratories that bridge catalysis and electro-catalysis will be discussed, ranging from oxidative dehydrogenation of alkanes to oxygen reduction reaction in fuel cells.

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**Abstract**. Methanotrophic bacteria containing particular methane monooxygenase (pMMO), a Cu-containing enzyme, or soluble methane monooxygenase (sMMO), an iron-metalloenzyme can oxidize methane to methanol selectively at ambient conditions 1. The zeolite Cu-ZSM-5 was reported to activate the methane C-H bond—with a homolytic bond dissociation energy of 104 kcal/mol— at temperatures as low as 120 °C 2 after pretreatment in O2 3. The reactive copper species are believed to contain extra-lattice oxygen, and in the case of Cu-ZSM-5, to be a mono-µ-oxo-dicopper complex ([Cu—O—Cu]2+) 4. Although a correlation was found between the concentration of mono-µ-oxo-dicopper species and the amount of methanol produced by Cu-ZSM-5 5, no such correlation was found for other zeolites that produce methanol such as Cu-mordenite and Cu-ferrierite 2. We have recently showed methanol production on copper (II) exchanged small pore zeolites including SSZ-13 (CHA), SSZ-16 (AFX) and SSZ-39 (AEI) with yields as high as 39 µmol CH3OH/g and CH3OH/Cu ratios up to 0.09 (the largest reported to date).6 Here, copper species in these small pore zeolites were investigated with UV–vis and Raman spectroscopy after O2-treatment at a temperature of 450 °C. No evidence of mono-µ-oxo-dicopper species was found in the spectra of Cu-SSZ-13,Cu-SSZ-16 and Cu-SSZ-39 6, however Cu—Oextralattice vibrations at 574 cm-1 were detected in Raman spectra of Cu-SSZ-13 and Cu-SSZ-39 zeolites which is indicative of a different CuxOy active species responsible for methanol production in small pore zeolites.

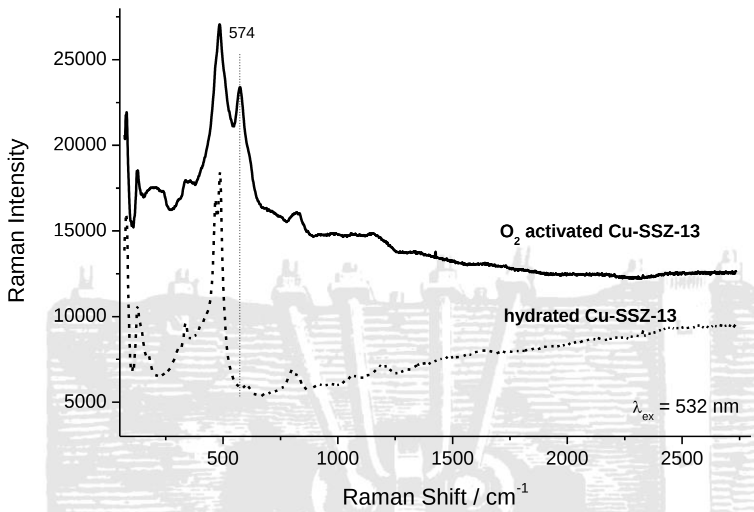


Figure 1. Comparison of Raman spectra taken before (dashed line) and after (solid line) O2-treatment of Cu-SSZ-13 (Si/Al=12, Cu/Al=0.45) at 450 °C for 2 h

**References.**


1. Hanson, R. S.; Hanson, T. E., Methanotrophic Bacteria. Microbiological Reviews 1996, 60, 439-471.
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3. Groothaert, M. H.; Smeets, P. J.; Sels, B. F.; Jacobs, P. A.; Schoonheydt, R. A., Selective Oxidation of Methane by the Bis(mu-oxo)dicopper Core Stabilized on ZSM-5 and Mordenite Zeolites. Journal of American Chemical Society 2005, 127, 1394-1395.
4. Woertink, J. S.; Smeets, P. J.; Groothaert, M. H.; Vance, M. A.; Sels, B. F.; Schoonheydt, R. A.; Solomon, E. I., A [Cu2O]2+ core in Cu-ZSM-5, the active site in the oxidation of methane to methanol. Proceedings of the National Academy of Sciences of the United States of America 2009, 106 (45), 18908-13.
5. Beznis, N. V.; Weckhuysen, B. M.; Bitter, J. H., Cu-ZSM-5 Zeolites for the Formation of Methanol from Methane and Oxygen: Probing the Active Sites and Spectator Species. Catal. Lett. 2010, 138 (1-2), 14-22.
6. Wulfers, M. J.; Teketel, S.; Ipek, B.; Lobo, R. F., Conversion of Methane to Methanol on Copper Containing Small Pore Zeolites and Zeotypes. Chem Commun 2015, xx, xx-xx.