Southwest Catalysis Society

Fall Symposium Series

Thursday December 8, 2016 @ University of Houston

Reception/Dinner: 6:00 – 7:30 PM; Seminar 7:30 – 8:30 PM

Combined Modeling and Experimental Studies of Oxidation Catalysis in MOFs and Zeolites

Prof. Randall Q. Snurr

Northwestern University

Department of Chemical & Biological Engineering

Zeolites and metal-organic frameworks (MOFs) have long been discussed as potential enzyme mimics for highly selective catalysis, and recent advances in synthesis are moving the field ever closer to this goal. Molecular-level modeling can play an important role in this development. MOFs provide a flexible platform for incorporating well-defined catalytic sites into carefully controlled environments. The talk will highlight examples of such systems, including nanoparticles enshrouded by MOF coatings. Through collaborations, a tight integration of modeling and experiment has provided new insights into these systems. Incorporation of titanium into zeolites also provides well controlled active sites for oxidation catalysis. Recently, with experimental colleagues, we have examined epoxidation of alkenes with hydrogen peroxide in TS-1 in both the liquid and gas phases. The use of gas-phase hydrogen peroxide may open up opportunities for generating new active oxygen species.

Randy Snurr is the John G. Searle Professor of Chemical and Biological Engineering at Northwestern University. He holds BSE and PhD degrees in chemical engineering from the University of Pennsylvania and the University of California, Berkeley, respectively. From 1994-95, he performed post-doctoral research at the University of Leipzig in Germany supported by a fellowship from the Alexander von Humboldt Foundation. Other honors include a CAREER award from the National Science Foundation, the Leibniz professorship at the University of Leipzig in 2009, and the 2011 Institute Award for Excellence in Industrial Gases Technology from the American Institute of Chemical Engineers. He has also been named a Highly Cited Researcher by Thomson Reuters. He served as a Senior Editor for the *Journal of Physical Chemistry* and is currently on the editorial boards of *Adsorption*, *Adsorption Science & Technology*, *Chemistry of Materials*, *Current Nanoscience*, and the *Journal of Molecular Catalysis A*. His research interests include development of new nanoporous materials for energy and environmental applications, molecular simulation, adsorption separations, diffusion in nanoporous materials, and catalysis.

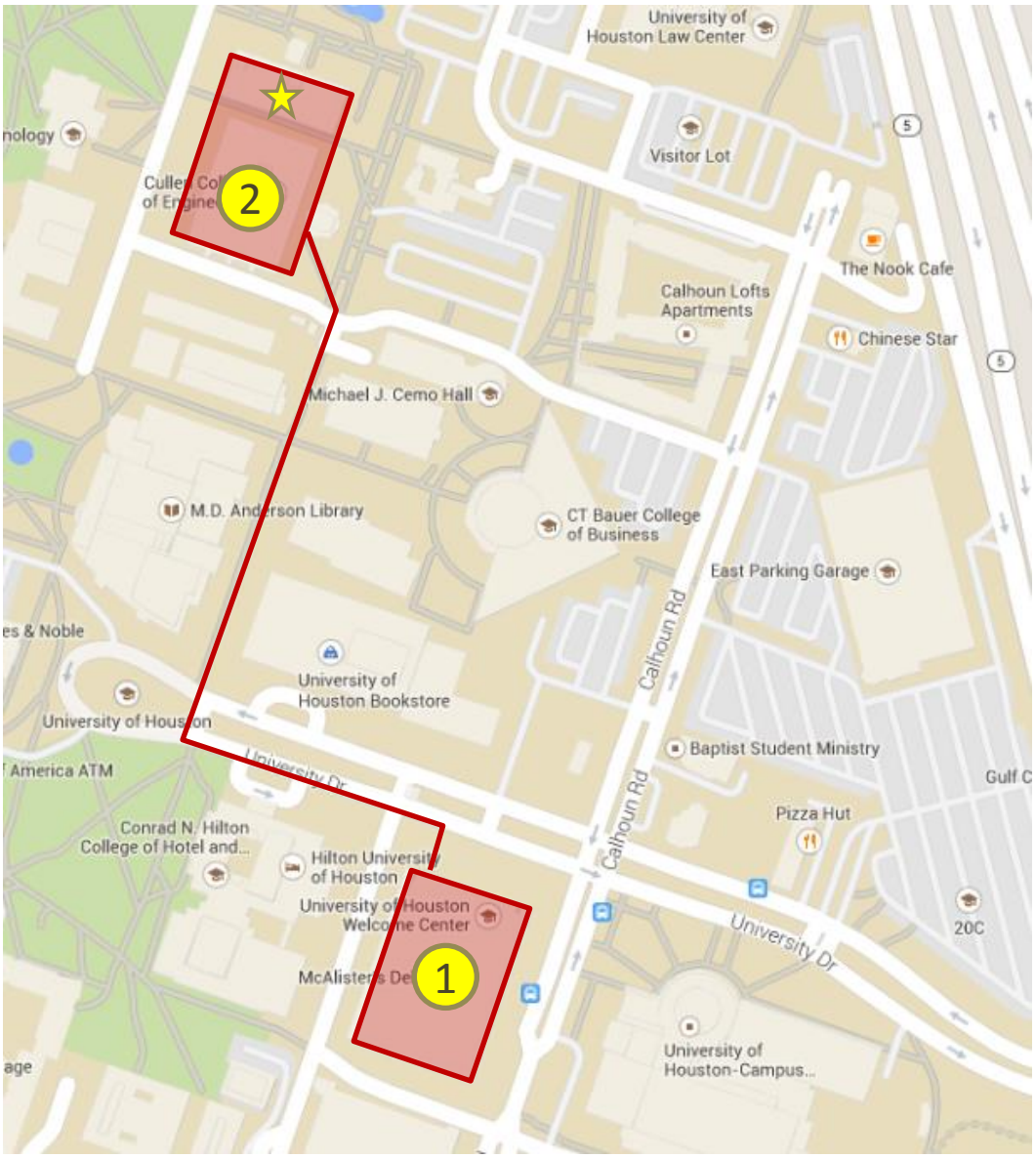
Location: University of Houston, Dept. Chemical Engineering

Reception: Engineering Building 1 Commons (1st Floor)

Seminar: Engineering Building 2, Room W122

Registration Fee: $30 Non-member, $20 Member, $10 Students/Postdocs

University of Houston Map: Parking and Event Location



1 **Parking garage:** 4400 University Drive, Houston, TX 77204

2 **Reception:** Engineering Building 1 (commons, 1st Floor)

★ **Seminar Room:** W122, Engineering Building 2

— Walking path from parking garage to event site