

## Matthew Neurock

Matthew Neurock is the Alice M. and Guy A. Wilson Professor of Chemical Engineering and Professor of Chemistry at the University of Virginia. He joined the faculty in chemical engineering at the University of Virginia in 1995 after receiving his PhD from the University of Delaware and working as a postdoctoral fellow at the Eindhoven



University of Technology in the Netherlands and at the DuPont Corporate Catalysis Center. He has received various awards for his research in computational catalysis and molecular reaction engineering, including the 2007 R. H. Wilhelm Award in Chemical Reaction Engineering, the 2007 Robert A. Moore Award, and the 2005 Paul H. Emmett Award in Fundamental Catalysis from the North American Catalysis Society. He was also a visiting professor at Southampton University in 2009, a Distinguished Visiting Professor at the University of Montpellier in 2007, and the Johansen-Crosby Lecturer at Michigan State University in 2006. He has received an NSF Career Development Award, a

DuPont Young Faculty Award, and a Ford Young Faculty Award. He has coauthored more than 184 papers, two patents, and two books. His most recent book was *Molecular Heterogeneous Catalysis: A Conceptual and Computational Approach*. He is an editor of the *Journal of Catalysis* and serves on the editorial boards of *Applied Catalysis A: General* and *Electrocatalysis* and on the international advisory board of *ChemCatChem*.

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## Richard S. H. Mah Lectures

**2005** James Wei, Princeton University

**2006** John H. Seinfeld, California Institute of Technology

**2007** Bernhard Ø. Palsson, University of California, San Diego

**2008** Glenn H. Fredrickson, University of California, Santa Barbara

## Richard S. H. Mah

Richard S. H. Mah was a leader in the movement to incorporate digital computing methods and their applications into chemical engineering practice and education.



Born in China, Mah received a BSc from England's University of Birmingham and a PhD from Imperial College in London, both in chemical engineering. After a two-year postdoctoral appointment at the University of Minnesota, he spent five years each with Union Carbide Corporation and the Exxon Math and Systems Company. From 1972, when he joined Northwestern, until 1995, Mah dedicated his life to chemical engineering education and research. He authored many papers in the technical literature as well as the influential monograph *Chemical Process Structure and Information Flows* (1993). Mah held leadership positions in the Computing and Systems Technology division of the American Institute of

Chemical Engineers (AIChE). He was a founding member and later president of CACHE, a nonprofit corporation dedicated to furthering the use of computer aids for chemical engineering. Among his many professional accolades were the Youden Prize of the American Society for Quality Control (1986), the AIChE Computing in Chemical Engineering Award (1981), and the Ernest Thiele Award of the Chicago Section of AIChE (1990). He became a fellow of the AIChE in 1985. His last formal scholarly accomplishment was a DSc in chemical engineering from the University of London Imperial College of Science and Technology in 1993.

The Richard S. H. Mah Lectures on Modeling and Computation in Chemical and Biological Engineering have been established through the generosity of the Mah family to honor the memory of Richard S. H. Mah and his contributions to Northwestern University, its Department of Chemical and Biological Engineering, and the profession of chemical engineering. In particular, the lectures are meant to honor Mah's role as a champion of introducing digital computing into modern chemical engineering. Each year a recognized leader in the field is invited to address topics that will cover diverse applications within the broad area of modeling and computation in chemical and biological engineering and will also appeal to individuals working in a wide range of disciplines.



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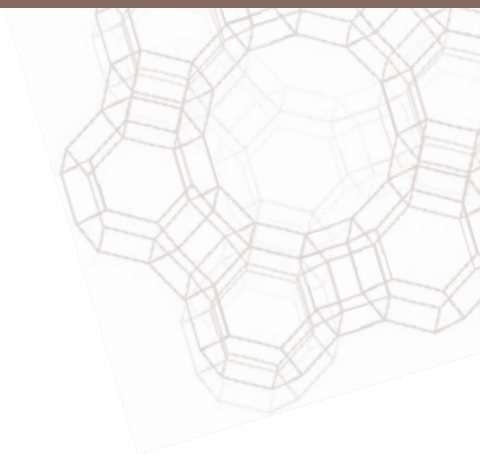
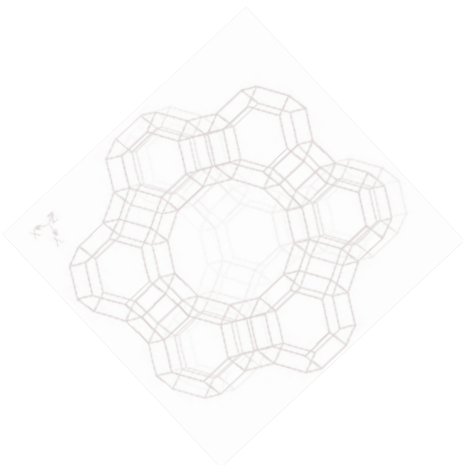
# Richard S. H. Mah Lectures

on Modeling and Computation in  
Chemical and Biological Engineering

Presented by

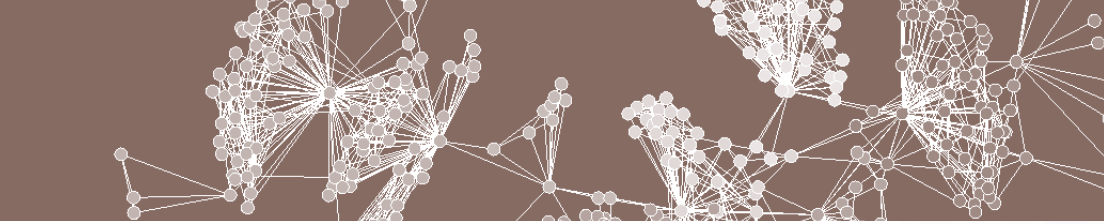
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Robert R. McCormick School of  
Engineering and Applied Science  
Northwestern University

**Department of Chemical and  
Biological Engineering**



The Department of Chemical and Biological Engineering  
in the Robert R. McCormick School of Engineering and  
Applied Science at Northwestern University

cordially invites you to the

**Fifth Annual**

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on Modeling and Computation in  
Chemical and Biological Engineering

Presented by

**Matthew Neurock**

Alice M. and Guy A. Wilson Professor of Chemical Engineering and  
Professor of Chemistry at the University of Virginia

## **Engineering Molecular Transformations**

**Wednesday, October 14, 2009**

**Lecture 4:30 p.m.**

*Pancoe Auditorium, Room 1101*

*Arthur and Gladys Pancoe Life Sciences Pavilion*

*2200 Campus Drive, Evanston, Illinois*

*Reception to follow in the Einstein Bros. Bagels meeting area*

*Parking is available after 4 p.m. in the parking lot east of the  
Pancoe Life Sciences Pavilion*

## **Elucidating the Catalytic Sites and Mechanisms That Control Hydrocarbon Oxidation**

**Thursday, October 15, 2009**

**Lecture 4 p.m.**

*Pancoe Auditorium, Room 1101*

*Arthur and Gladys Pancoe Life Sciences Pavilion*

*2200 Campus Drive, Evanston, Illinois*

[www.chem-biol-eng.northwestern.edu](http://www.chem-biol-eng.northwestern.edu)

# Engineering Molecular Transformations

**Wednesday, October 14**

**Lecture 4:30 p.m.; reception to follow**

Future strategies for energy production will require processes and materials that can efficiently convert sustainable resources into fuels and chemicals. While nature's enzymes elegantly integrate highly active centers with adaptive nanoscale environments to control the catalytic transformation of molecules to specific products, they are difficult to incorporate into large-scale industrial processes and limited in terms of their stability. The design of more robust heterogeneous catalytic materials that can mimic enzyme behavior, however, has been hindered, however, by our limited understanding of how such transformations proceed over inorganic materials. Tremendous advances in *ab initio* theoretical methods and high-performance computing over the past two decades provide unprecedented ability to track these molecular transformations and how they proceed at specific sites and within particular environments. This information, together with the unique abilities to follow such transformations spectroscopically, is enabling the design of unique atomic surface ensembles and local reaction environment that can efficiently catalyze specific molecular transformations. This talk presents the advances within chemistry and chemical engineering that have enabled this evolution of molecular engineering and discusses their application to energy conversion strategies and chemical syntheses.

# Elucidating the Catalytic Sites and Mechanisms That Control Hydrocarbon Oxidation

**Thursday, October 15**

**Lecture 4 p.m.**

An atomic-scale understanding of the active sites that control catalytic and electrocatalytic systems and their local reaction environment could lead to tremendous breakthroughs in our ability to design more active and selective materials. While the intrinsic chemical bonds that are formed and broken as part of the operative catalytic cycle are critical, the influence of defect sites, alloy composition and specific arrangement, support effects, coadsorbed intermediates, surface coverage effects, and solution can be just as important. An understanding of how these features form and their influence on the reaction kinetics could aid the design of next-generation materials with improved catalytic performance. *Ab initio* quantum mechanical methods have reached the stage where they can be used to model the atomic structure along with the local molecular topography of proposed active sites and establish the influence of their environment on their catalytic reactivity. The results from theory can subsequently be integrated with atomic-scale simulations in order to track individual transformations of molecules over catalytic substrates, thus connecting catalytic structure with performance. This allows for an “*in silico*” approach that can tailor these structural features toward the control of specific catalytic properties. This talk describes the application of theory and simulation to the partial oxidation of methane over supported metal particles and the electrocatalytic conversion of oxygenates over metal and alloys surfaces. Theory is coupled with kinetic and dynamic simulations to interrogate the nature of the catalytically active surfaces sites and ensembles and the influence of surface coverage and solution, as well as electrochemical potential for these two processes.