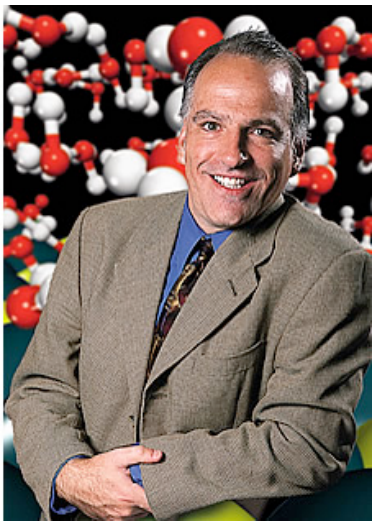
Physical Chemistry Seminar

Tuesday, March 11, 2014 | **11:00 am** | **Room 1315 Chemistry Building**

Engineering Molecular Transformations over Supported Catalysts for Sustainable Energy Conversion



Professor Matthew Neurock

Departments of Chemistry & Chemical Engineering
University of Virginia

Host: Professor JR Schmidt

Future strategies for energy production will undoubtedly require processes and materials that can efficiently convert sustainable resources into fuels and chemicals. While nature's enzymes elegantly integrate highly active centers together with adaptive nanoscale environments in order to exquisitely 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 by our limited understanding of how such transformations proceed over inorganic materials. The tremendous advances in ab initio theoretical methods, molecular simulations and high performance computing that have occurred 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 nanoscale reaction environment that can efficiently catalyze specific molecular transformations. This talk discusses recent advances in computational catalysis and their application to engineering molecular transformations for energy conversion and chemical synthesis. More specifically, we will discuss the sites and nanoscale reaction environments necessary to carry out specific bond making and breaking reactions important in conversion of renewable feedstocks and the design of 2D and 3D environments necessary to carry out such transformations. The talk discusses applications to selective oxidation and hydrogenation of oxygenates over supported metal catalysts for biomass conversion, zeolite catalyzed C-C bond formation paths in the production of fuels and chemicals and electrocatalytic oxidation/reduction processes for fuel cells.

Refreshments will be available prior to the seminar at 10:45 a.m. outside room 1315

Graduate Students may meet with the speaker at 1:00 p.m. in Room 8335