

Karl Sohlberg

Associate Professor, Theoretical and Computational Chemistry, Tel: 215-895-2653, Fax: 215-895-1265, E-mail: sohlbergk@drexel.edu, Webpage: <http://www.chemistry.drexel.edu/people/sohlberg.asp> (b. 1964), B.S. 1985, University of Vermont; Ph.D. 1993, University of Delaware; Postdoctoral fellow, Brigham Young University; Postdoctoral fellow, The Johns Hopkins University; Oak Ridge Associated Universities Postdoctoral fellow, Oak Ridge National Lab.

Current Research

My research may be broadly classified as computational and theoretical materials-related chemistry. Under this umbrella I have two major research thrusts. The first major research thrust is in **complex catalytic materials**. The second major research thrust is in **mechanical and electrical molecular devices**.

Complex catalytic materials

Catalysis is a critical factor in energy efficiency and clean energy. It is the enabling technology for petroleum production, for control of the final gaseous emissions from petroleum combustion, and for the industrial production of bulk and fine chemicals. Since the global utilization of catalysts is enormous, even incremental improvements in these catalysts would translate into vast reductions in energy consumption and effluent production. An atomic-level understanding of catalytic materials would be a very powerful tool to aid the selection of improved catalysts and the optimization of their properties. At present, however, there is very limited information on the atomic configurations of the active sites, their electronic structure, and the influence of these factors on efficiency and durability. This lack of atomic-scale details about the nature of catalytic materials is the key roadblock to improved catalyst design. Without such information, the development of improved catalysts is heavily empirical. It is the ultimate goal of my research program in complex catalytic materials to deliver, for the first time, an atomic-scale description of catalysts that can illuminate the path to precision atomic-scale engineering of new catalysts for optimum performance.

Important results from this research include:

- a detailed atom-by-atom description of the transformation of γ - to θ -alumina (1).
- a demonstration of how a subtle difference between the distribution of bulk defects in two ubiquitous catalytic support materials, γ - and η -alumina, gives rise to qualitatively different surface chemistries and consequently different catalytic activities (2).
- An explanation of the anomalous structure of Pt₃ clusters observed on the surface of Pt/ γ -alumina catalysts (3).
- developing a mathematical model that directly links atomic-scale surface structure of heterogeneous catalysts to macroscopic measurements of surface conductance (4).

Excellent collaborations bring the world-class electron microscopy facilities of Oak Ridge National Laboratory to the project. Current and past funding comes from USDoe, NSF, NATO, NCSA and DuPont Inc.

Molecular devices

Nanotechnology promises engineered devices constructed from just one or a few molecules, a technology with potentially staggering impact. Applications are envisioned in medicine, molecular electronics based information processing systems, and information gathering and monitoring for defense, space science, and other extreme environments. Molecular turbines

pumping streams of gas one molecule at a time, minuscule valves delivering drugs with unprecedented site and dose specificity, pinhead scale computer disks storing libraries of information, and extremely sensitive artificial olfaction for contraband detection,



are all theoretically possible. To facilitate the *systematic* design and refinement of functional molecular devices, it would be desirable to have available robust and validated modeling techniques. The ultimate goal of the program is to develop design-engineering tools – “recipes” for nano-devices by design. Key results from this research include:

- a quantum mechanical explanation for the observation of strong substituent dependence of nonlinear I/V characteristics in molecular electronic junctions (5). A news item about this research subsequently appeared in the Feb. 2002 issue of *Materials Today*.
- a computational scheme for modeling switchable rotaxane systems, and the successful application of this scheme to experimentally realized examples (6).

Related Publications

- (1) Shu-Hui Cai, Sergey N. Rashkeev, Sokrates T. Pantelides and Karl Sohlberg, “Atomic Scale Mechanism of the Transformation of γ -Alumina to θ -Alumina,” *Phys. Rev. Lett.*, **89**, 235501 (2002).
- (2) Karl Sohlberg, Stephen J. Pennycook, and Sokrates T. Pantelides, “Surface reconstruction and the difference in surface acidity between γ - and η -alumina,” *J. Am. Chem. Soc.*, **123**, 26 (2001).
- (3) Karl Sohlberg, Sergey Rashkeev, Albina Y. Borisevich, Stephen J. Pennycook and Sokrates T. Pantelides, “Origin of anomalous Pt-Pt distances in the Pt/alumina catalytic system,” *ChemPhysChem*, **5**, 1893-1897 (2004).
- (4) Shuhui Cai, Monica Caldararu, Viorel Chihaiia, Cornel Munteanu, Cristian Hornoiiu and Karl Sohlberg, “Possible dual-charge-carrier mechanism of surface conduction on γ -alumina,” *J. Phys. Chem. C*, **111**, 5506-5513 (2007).
- (5) Nikita Matsunaga and Karl Sohlberg, “The substituent effect on non-linear I/V characteristics in a two-terminal molecular electronic device,” *J. Nanosci. Nanotech.*, **1**, 275 (2001).
- (6) Xiang Zheng and Karl Sohlberg, “Modeling of a Rotaxane-based Molecular Device,” *J. Phys. Chem. A*, **107**, 1207 (2003).