



## Graduate studies in chemical kinetics and catalysis at Stevens Institute of Technology

Two PhD graduate students can join my research group in the fall of 2009. The main research area is reaction mechanism studies on surfaces of solid catalysts for petroleum refining and chemical industries. Research methodology involves both experimental and theoretical work, and students would be encouraged to explore both areas, but can, obviously, choose to focus on one of them.

### *Experimental studies:*

- Preparation of metal and metal oxide solid (heterogeneous) catalysts;
- catalyst testing with special emphasis on collecting kinetic data;
- catalyst characterization with special emphasis on infrared and Raman spectroscopies of catalyst surface species.

### *Theoretical studies:*

- kinetic modeling;
- Density Functional Theory (DFT) quantum-chemical calculations.
- Monte Carlo molecular simulations.

### *Research methodology:*

An iterative cycle of experimental catalyst characterization and testing combined with density-functional theory (DFT) calculations of surface species provides information for the development of reaction mechanisms. Experimental information establishes the basis for the selection of models and the level of theory for DFT calculations and then, in turn, results of the DFT calculations allow to deconvolute and better interpret experimental data. Experimental and theoretical results on the modes of adsorption, energetics and reactivity of surface species can be consolidated into a traditional kinetic model for the description of observable reaction rates. For more detailed studies on the connection between nano-scale chemistry and macroscopic properties, results of DFT calculations can be combined with Monte Carlo simulations.

Usual objectives of mechanistic studies: (1) catalyst development, (2) process development or optimization, (3) improvement of process control.

### *Current projects:*

- (1) Fischer-Tropsch synthesis to light hydrocarbons and to diesel fuel is funded by the US Department of Defense. Additional joint proposal with Columbia University, BASF and USDA is pending at the National Science Foundation (NSF).
- (2) Selective methane activation to chemical feedstocks and fuels.
- (3) Catalysis over gold nanoparticles.

***Admission:***

[GRE](#) and [TOEFL](#) (for non-English speaking students) test results are usually required for admission. For students admitted as a Research Associate or a Teaching Assistant, tuition will be paid. In addition a stipend of about \$1,800 per month will be provided. Stevens Institute is a small private university located next to Manhattan on the other side of the Hudson River ([map link](#)). Living expenses, especially housing, in the New York area are high. But judging from the experience of current students, the stipend is sufficient to survive. The Stevens School of Engineering was ranked to be 80-th across all of the US last year ([ranking link](#)), but my group will, obviously, strive for much higher ranking in catalysis research.



*View of the entrance to the Stevens Institute of Technology in Hoboken and Manhattan across the Hudson River.*

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