STEVENS INSTITUTE of TECHNOLOGY
THE INNOVATION UNIVERSITY

University Seminar Series

Sponsored by Nanotechnology Seminar Program

Discovery of nanostructured catalytic materials for automotive applications using a combined approach of informatics, modeling, and experiment

Dr. George B. Fitzgerald

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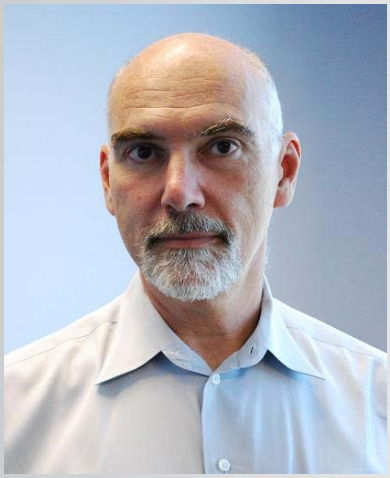
San Diego, California



ABSTRACT

Increasing regulatory environmental requirements and consumer trends are forcing corporations to develop environmentally friendly alternatives to the status quo, and the automobile industry stands out as a highly visible example because of tailpipe emissions. Improved formulations for catalytic converters alleviate pollutants in a number of ways. Foremost, of course, they reduce CO, NO_x, and hydrocarbon emissions. In the long term, however, the internal combustion engine may be replaced with 'zero emission' technologies, such as fuel cells, which will require an entirely different set of catalysts. The number of materials that must be considered during discovery of nanostructured catalysts increases combinatorially with evaluation of multiple compositions and processing steps and usually reaches millions. Methods are needed that allow researchers to better understand nanotechnology and focus their efforts in the most promising areas. This presentation will examine how informatics and nanoscale modeling are being combined with experiment to reduce the time and cost required to discover new optimum materials. Two commercial case studies will be presented: (1) Selective catalytic reduction to reduce NO_x emissions and (2) Reducing the noble metal content of catalysts with platinum nanoparticles in fuel cells through doping with transition metals. The use of a data management system helped to increase material evaluation throughput by 100-fold.

BIOGRAPHY

George Fitzgerald received a B.S. in Chemistry from Case Western Reserve University in 1980. He received his Ph.D. from the University of California, Berkeley in 1984 where he studied the development and application of ab initio quantum chemistry under the direction of Prof. H.F. Schaefer. He joined Accelrys Software, Inc., in 1987 as the director of the Catalyst Consortium, a group of corporations and universities dedicated to developing new computational methods for catalysis. Today he is an Advisory Scientist at Accelrys, working in collaboration with corporate and government customers on catalytic research problems using molecular modeling and informatics. His research interests include nanotechnology, alternative energy, and evolutionary computing methods. He has chaired and organized multiple national and international research conferences. Most recently, he organized a symposium on “Applications of Computational Methods to Environmentally Sustainable Solutions” at the National Meeting of the American Chemical Society in March 2012.

EVENT DETAILS

DATE:
Wednesday Feb. 20, 2013

TIME:
11:00 AM

LOCATION:
Babbio Center, Room 122
Stevens Institute of Technology

ATTENDANCE:
This event is open to Stevens’ Faculty, Students, Staff, and Invited Guests

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