Chemical and Petroleum Engineering

Edward Maginn

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Edward Maginn received his BS in chemical engineering from Iowa State University and his PhD in chemical engineering from the University of California, Berkeley. Prior to attending graduate school, he worked as a process engineer for Procter and Gamble. He has been on the Notre Dame faculty since 1995 and currently holds the Dorini Family Chair of Energy Studies in the Department of Chemical and Biomolecular Engineering. He is also the chair of the department. He has won a number of awards, including the Early Career Award from the Computational Molecular Science and Engineering Forum of the American Institute of Chemical Engineers, the American Society of Engineering Education Dow Outstanding New Faculty Award, the BP College of Engineering Outstanding Teacher Award and the NSF Career award. He is a Fellow of the American Association for the Advancement of Science and is a trustee of the CACHE Corporation. His research focuses on the development and use of atomistic molecular dynamics and Monte Carlo simulation methods to study the thermodynamic and transport properties of materials, with special emphasis on ionic systems important in energy storage and use.

"Computational Design of New Materials for Energy Efficient Separations"

Abstract

It has been estimated that chemical separation technologies such as distillation account for 10-15% of the world's energy consumption. As a consequence, the National Research Council has called for the development of alternatives to distillation to meet the Energy Intensity of Chemical Processing Grand Challenge. There are two approaches that can be taken. First, chemical transformations can be made more selective, so that little to no downstream separation is required. Second, separations can be affected by materials instead of heat. Examples include membranes, sorbents, or solvents. To develop new materials capable of achieving these objectives, a detailed understanding of the thermodynamics, reactivity and transport properties of the molecules to be separated and the catalysts and mass separating agents used is needed.

In this talk I will focus on how we are developing and applying advanced molecular simulation techniques to study how new membranes and solvents can be developed to enable more energy efficient separations. In the first part of the talk, I will focus on ionic liquids designed to preferentially separate CO2 from air, methane and hydrogen. Permeabilities / separation factors are computed for ionic liquids confined in membranes and in nanoporous media. The solubility of chemically reacting ionic liquids is computed directly using a combination of quantum and classical modeling approaches. A new reactive Monte Carlo (RxMC) method is described that enables the direct calculation of the reactive absorption isotherm as a function of pressure. The underlying structure of these reactive ionic liquids is described via simulations; quantitative agreement with experimental x-ray scattering structure functions is obtained, but the simulations also provide three-dimensional information on the organization in the liquid that is not available from the experiments. In the second part of the talk, I show how the RxMC method can be used to predict how the condensed phase or local environment shifts the equilibrium distribution of products for other reactions. Extreme nanoconfinement (such as that present in zeolites or other porous catalysts) can shift the equilibrium distribution of reacting xylene isomers to the desired products.

Tuesday, April 10th | 10:00 – 10:50AM | Spahr Auditorium