Computational Design of New Materials for Separations and Energy Storage

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**ABSTRACT** Chemical separation technologies such as distillation account for tremendous amount 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. In the first part of this talk, I will focus on ionic liquid solvents 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.

Energy storage technologies such as rechargeable batteries are key enablers of renewable energy sources such as wind and solar. The development of “beyond lithium ion” batteries, such as multi-valent and Li-sulfur batteries, relies upon the development of new electrolytes. In the second part of the talk, I will describe our work as part of the Joint Center for Energy Storage team on understanding the structure and dynamics of electrolytes used in these advanced batteries.

**BIO** Dr. 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 and was formerly the Associate Dean for Academic Programs in the Notre Dame Graduate School. He is the Senior Editor and founder of the Springer Nature series Molecular Modeling and Simulation: Applications and Perspectives. 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 for Engineering Education Dow Outstanding New Faculty Award, the BP College of Engineering Outstanding Teacher Award and the National Science Foundation Career award. He is a Fellow of the American Association for the Advancement of Science and the American Institute of Chemical Engineers and is a trustee and vice-president of the non-profit 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 and environmental.