# POSTDOCTORAL POSITIONS IN MOLECULAR MODELING
# UNIVERSITY OF NOTRE DAME

The Molecular Engineering and Simulation Lab in the Department of Chemical and Biomolecular Engineering at the University of Notre Dame (USA) has immediate openings for three postdoctoral research assistants under the direction of Prof. Edward J. Maginn.

Ionic Liquids Research (two openings)

One of the ionic liquids projects is focused on the development of new ionic liquids for use in post-combustion $CO_2$ capture. The other project deals with developing new ionic liquids for application in geothermal energy generation. Both projects seek to use molecular modeling to design new ionic liquid materials with properties tailored for the particular activities. The positions will require the development and application of atomistic simulation methods for calculating the thermodynamic and transport properties of complex ionic liquid systems. Successful candidates will be expected to work closely with experimental groups at Notre Dame and in industrial partner labs to help translate their computational work into results useful to experimentalists. Both projects are sponsored by the US Department of Energy.

Confined Colloids Simulation (one opening)

This project is concerned with understanding the structural and dynamic properties of colloids under extreme confinement. It is a collaboration with Prof. Elaine Zhu's group at Notre Dame, who have used advanced imaging techniques to directly examine individual colloid particle motion under confinement. The goal is to develop accurate and efficient computational methods that enable these systems to be simulated to help understand and interpret their experimental results. Support is provided by Notre Dame's Center for Computational Research (crc.nd.edu) and interaction with staff scientists and other affiliates within the Center is expected.

Successful candidates will be highly motivated, able to work with graduate students and possess good written and spoken English skills. All positions will involve the use of particle-based simulation methods (molecular dynamics, Monte Carlo, Brownian dynamics). The positions may also require the use of *ab initio* calculations to develop force fields. The ability to develop and apply new advanced simulation methods that enable efficient calculation of relevant properties is also desirable.

Candidates must have a Ph.D. degree in chemical engineering, chemistry, physics, or a related field. Expertise in molecular dynamics, Monte Carlo, electronic structure calculations and / or force field development is highly desired. A competitive salary and benefit package is provided, along with access to state-of-the-art computational facilities. as part of Notre Dame's Center for Research Computing (crc.nd.edu) and the Northwest Indiana Computational Grid (www.nwicg.org).

Applications with a curriculum vita and a brief statement of research should be sent by email (pdf format strongly encouraged) to Edward Maginn (ed@nd.edu). Names and contact information for three references familiar with the candidate's work should also be provided.