Professor Debra Bernhardt

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The Bernhardt research group is interested in the study of matter using theoretical and computational methods that can ultimately be used to address a wide range of practical problems. Applications of interest include transport in nanopores, fluctuations in nanoscale systems, melting, solubility, separation of gases, lubrication, design of ionic liquids, design and assessment of materials for energy conversion and storage, carbon dioxide sequestration and catalysis. The group has world leading expertise in various theoretical and computational methods ranging from quantum chemical calculations to the statistical mechanics of nonequilibrium systems, access to high performance computing facilities and an international team of collaborators.

Transport in nanoporous systems

Nanoporous solids are used as adsorbents in pollution control, industrial separations, storage of fluids and catalysis. Simulations can be used to assist in the design of better materials, and to understand the fundamental nature of the adsorption and transport processes. One of the key factors determining flow of fluids through nanopores is their stick or slip behaviour near the walls. We have recently developed a new approach for studying this behaviour that should be more efficient for complex systems.

Computational studies of ionic liquids

Ionic liquids have exceptional solvation properties and electrical conductivity, meaning they have a wide range of industrial applications. By combining different ions, ionic liquids can be designed to optimize their properties. However, the science of ionic liquids is new and therefore prediction of their properties is problematic. To address this, we are taking advantage of recent developments in nonequilibrium statistical mechanics to create efficient algorithms to determine key properties of ionic liquids.

Statistical mechanics of nonequilibrium fluids

Any system that is flowing, stirred, has a temperature gradient across it or is subject to an external field is in a nonequilibrium state. The properties of these systems are not well developed when the systems are far from equilibrium. In this project theory and computational methods will be used to expand our fundamental understanding of these systems.

Quantum mechanics for the design of new materials

New materials are required for solar energy applications, catalysis, adsorbents for pollutants, storage of fuels, new polymers, fuel cells etc. Quantum mechanics enables the properties of these materials to be predicted in an efficient and cost effective manner. Projects are available that will focus on the prediction of material properties using a range of computational quantum chemical methods.