Molecular Dynamics Simulations of Clathrate Hydrates

Saman Alavi

Department of Chemistry and Biomolecular Sciences, University of Ottawa

Knowledge of molecular level details of materials is critical in predicting their behaviour under different working conditions. While X-ray diffraction, NMR, and IR-Raman spectroscopies and other experimental techniques are the ultimate source of molecular information on the behaviour of a material, they are often limited by their spatial and time resolutions. Distance ranges of up to tens of nanometers and time ranges of up to microseconds are where molecular dynamics simulations are most useful and where they complement existing experimental methods and can predict a range of material properties, in many cases with a level of confidence comparable to experimental techniques. In this talk, I will give a brief introduction to clathrate hydrate materials and their characterization by experimental methods. Results of molecular dynamics simulations on these materials will be presented to showcase some of the unique molecular-level information obtained from simulations. Hydrogen bonding of guest molecules to the water framework, the determination of NMR lineshapes for linear guest molecules, and the effects of antifreeze proteins on the growth of clathrate hydrates will be discussed as examples.