Abstract

Ongoing advances and breakthroughs in synthesis and experimental characterization techniques yield increasing detailed molecular-level information about chemical and physical processes that is becoming increasingly difficult to decipher without the guidance of modeling. Molecular modeling and simulations have thus rapidly been permeating all branches of chemistry, physics, biology and engineering, not only because they may help interpret convoluted experimental data, but also because they ultimately allow for further educated experimental design over time-consuming and costly trial-and-error approaches. Our research program centers on the development and application of state-of-the-art molecular dynamics and quantum chemistry techniques for realistic simulations of (bio)chemical and (bio)physical processes, enabled by high-performance computing and typically validated against and/or motivated by top-notch experimentation. This presentation will provide an overview of our chemical modeling research program, with particular emphasis on a few select topics such as ligand delivery to porous protein active sites, magnetic materials for spin catalysis, carbon-based molecular electronics, guest molecule encapsulation and storage, wear-resistant transition metal-nitride thin films and nanoparticles for opto-electronics.