Simulation of ice formation in nanopores at low temperatures and pressures

Fernando Escobedo

The formation of ice plays a key role in many natural processes that are relevant to atmospheric pollution, cloud formation, and aerosol radiative cooling. For example, deposition nucleation, which occurs in cirrus clouds, involves the low temperature/low pressure freezing of water vapor upon contact with aerosol particles. However, the widely variable ability of aerosols to freeze vapor is not well understood and casts many questions on the mechanism by which these particles nucleate ice. This project aims to elucidate the mechanism of water's vapor-to-solid phase change during deposition nucleation by testing the role of surface morphology on aerosols' ice nucleation ability. Because aerosol particles are typically porous with both large and small pores, this study focuses on the freezing of water in nanopores. Understanding this phase change is important not only for its relevance to atmospheric processes but also at a fundamental level, as the phase behavior of water at very low temperatures and pressures is very complex. We plan to conduct molecular dynamic simulations to study the nucleation and growth of ice in nanopores of different sizes, chemistries and morphologies. These studies are complementary to current experimental work in Prof. Stroock's lab.