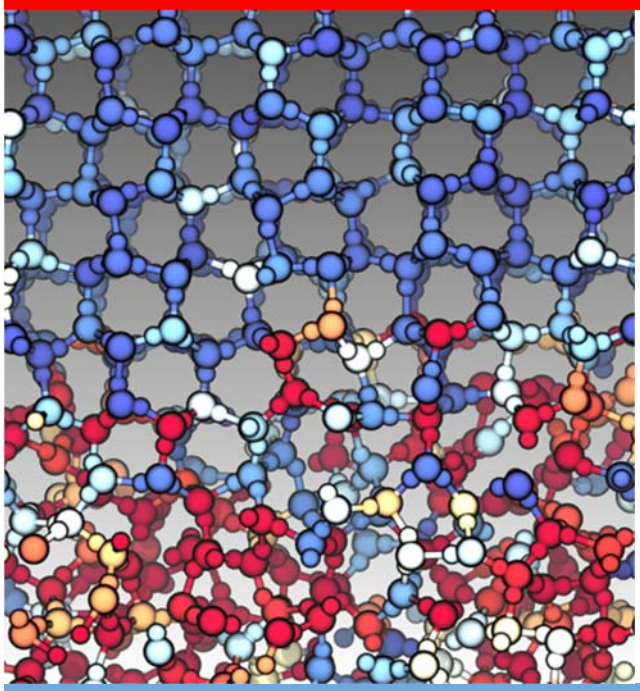
CHEMISTRY COLLOQUIUM

Guest Speakers:
Professor Christoph Dellago
University of Vienna
Faculty of Physics

Wednesday, September 18, 12:00pm
Hutchison Hall Room 140
Lander Auditorium
University of Rochester
Department of Chemistry



Title: "Machine learning in atomistic simulations: from reaction pathways to phase diagrams"

Abstract:: Atomistic computer simulations of processes occurring in condensed matter systems are challenging for several distinct but related reasons. For large systems, the accurate calculation of energies and forces needed in molecular dynamics simulations may be computationally demanding, particularly if electronic structure calculations are used for this purpose. Other difficulties arising in the dynamical simulation of condensed matter processes consist in detecting local structures characteristic for stable or metastable phases and in identifying important degrees of freedom that capture the essential physics of the process under study. In this talk, I will discuss how these problems can be addressed using machine learning approaches. I particular, I will focus on a computational study of water and ice based on a high-dimensional neural network potential trained with ab initio reference data. We have shown that Waals interactions are crucial for the formation of water's density maximum and its negative volume of melting. Our simulations have also revealed that nuclear quantum effects play an important role in modulating the thermodynamics stabilities of different phases of water.

Host: Professor Todd Krauss, email: todd.krauss@rochester.edu