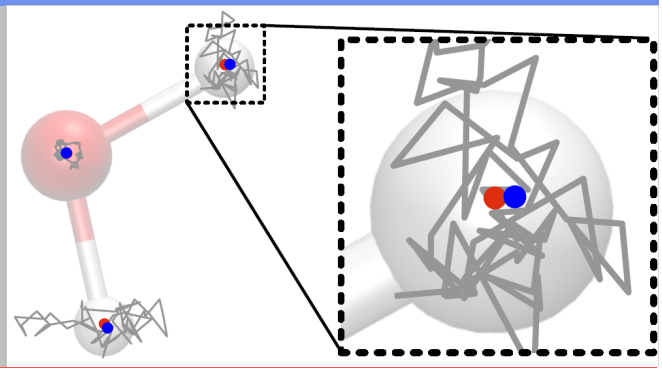
CHEMISTRY COLLOQUIUM

Professor Stuart Althorpe
University of Cambridge
Department of Chemistry

Wednesday, May 22, 12:00 pm
140 Hutchison Hall
Lander Auditorium
University of Rochester
Department of Chemistry



Title: "Simulating quantum dynamics in liquid water and ice"

Abstract: It is essential to treat atomic nuclei quantum mechanically if one wishes to simulate liquid water and ice using ab initio force fields. An established way to include such effects in simulations of static properties is to use Feynman path-integrals, in which each nucleus is represented as a 'ring-polymer' describing the delocalisation of the quantum Boltzmann statistics. This talk will address how to use ring-polymers to simulate dynamical properties in liquid water and ice, focusing on the the infrared spectrum.

Host: Professor Frank Huo • Email: huo@chem.rochester.edu