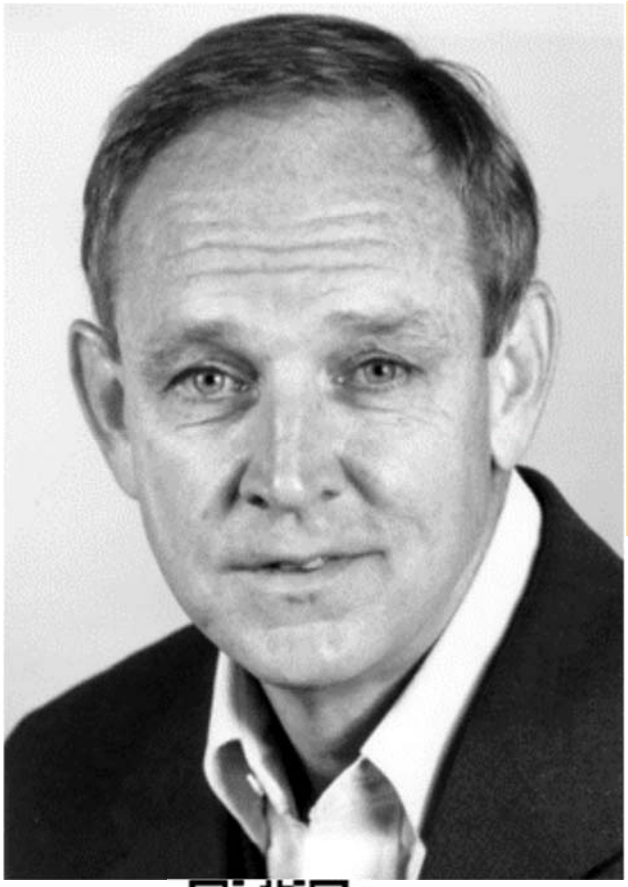
CHEMISTRY COLLOQUIUM



Guest Speaker:

Professor William H. Miller

UC Berkeley

Wednesday, September 27th, 12:00pm

Hutchison Hall Room 140

Lander Auditorium

University of Rochester

Department of Chemistry

"Classical Molecular Dynamics Simulations of Electronically Non-Adiabatic Processes"

Abstract:: A recently described symmetrical windowing methodology [*J. Phys. Chem. A* **117**, 7190 (2013)] for quasi-classical (SQC) trajectory simulations has been applied to the Meyer-Miller (MM) [*J. Chem. Phys.* **70**, 3214 (1979)] model for the electronic degrees of freedom in electronically non-adiabatic dynamics. The approach treats nuclear and electronic degrees of freedom (DOF) equivalently (i.e., by classical mechanics, thereby retaining the simplicity of standard molecular dynamics), and provides ``quantization'' of the electronic states through the symmetrical quasi-classical (SQC) windowing model. The approach is seen to be capable of treating extreme regimes of strong and weak coupling between the electronic states, as well as accurately describing coherence effects in the electronic DOF (including the de-coherence of such effects caused by coupling to the nuclear DOF). A survey of recent applications to a variety of problems is presented to illustrate the performance of the approach. Also described is a newly developed variation on the original SQC model (found universally superior to the original) and a general extension of it to obtain the full electronic density matrix (at no additional cost/complexity). It has also been pointed out that even though the MM classical vibronic Hamiltonian generates 'Ehrenfest dynamics', when this is processed via the SQC windowing methodology detailed balance is described correctly.

Host: Professor Frank Huo, email: pengfei.huo@rochester.edu