

PHYSICAL SEMINAR

“The dynamics of electrochemistry at a metal surface”

Guest Speaker:

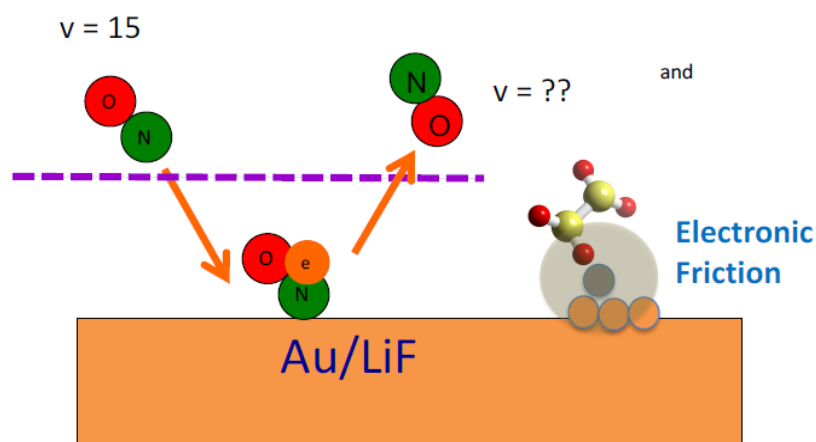
Professor Joseph Subotnik

University of Pennsylvania

Department of Chemistry



Scattering from a surface
nonadiabatically



Monday, March 26th, 4:00pm
Hutchison Hall Room 473
University of Rochester
Department of Chemistry

Abstract:

In recent years, there has been an explosion of computational research directed at understanding photochemistry and the exchange of electronic energy with nuclear motion and friction, many researchers have contributed to the development of hopping, spawning and mean-field algorithms. These efforts have been largely successful and today, we do have tools to predict the ultimate products of many photochemical reactions in solution (albeit with many CPU hours). That being said, there still remain many classes of reactions where we still do not have a predictive framework. In particular, for many electrochemical or especially photoelectrochemical processes, theoretical progress is sorely lacking. Whereas we know that, in most photochemical experiments, there is one energy sink and all the energy will be disbursed eventually as nuclear motion, for electrochemical problems there are two sinks of energy: the electronics of the electrode and the nuclear dynamics of the solvent. This predicament necessarily complicates theoretical progress. With that in mind, in this talk, I will discuss the simplest frameworks for quantifying and predicting dynamics near a metal surface and I will highlight both current applications and future theory challenges.

Host: Professor Ignacio Franco • Email: ignacio.franco@rochester.edu