



Department of Chemistry Seminar Series Fall 2022

Monday, November 7, 2022, 3:30 PM - **HS1 O112 (Health Sciences)**

Host: Fernando Uribe-Romo

Machine-learning-accelerated photodynamics simulations in complex environments towards new photomedicines



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Photochemical reactions are increasingly important for constructing value-added, strained organic architectures. Direct excitation and photoredox reactions typically require mild conditions to access therapeutic gases (e.g., carbon monoxide) and new synthetic methodologies. *A priori* design of photochemical reactions is challenging because degenerate excited states often result in competing reaction mechanisms to undesired products. Further, a lack of experimental techniques that provide atomistic structural information on ultrafast timescales (10^{-15} – 10^{-12} s) has limited general rules about these reactions. Computations, however, provide a path forward. I will discuss how my group has leveraged multiconfigurational complete active space self consistent field (CASSCF) calculations, non-adiabatic molecular dynamics, and machine learning (ML) techniques to understand reaction mechanisms and enumerate new reaction pathways. I will introduce our new open-access machine learning tool, Python Rapid Artificial Intelligence *Ab Initio* Molecular Dynamics (PyRAI²MD), which enables 100,000-fold longer simulations than current NAMD simulations with multiconfigurational quantum chemical methods. I will describe how PyRAI²MD has enabled the first ML-NAMD simulations with QM/QM (CAS/HF) training data. The presentation will explain the origins of the reactivities and selectivities of photochemical pericyclic reactions and CO-evolving reactions in aqueous environments.