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**Houk-Jung  
Organic Colloquium**

**Photodynamics simulations explain  
photochemical reactivity and selectivities  
towards strained molecules**

**Abstract:** Photochemical reactions are increasingly important for the construction of value-added, strained organic architectures. Direct excitation and photoredox reactions typically require mild conditions and permit access highly strained molecules and new synthetic methodologies. The *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) limits general 'chemical intuition' about these processes. Computations, however, provide a path forward. I will discuss how my group has leveraged state-of-the-art quantum mechanical calculations, non-adiabatic molecular dynamics, and machine learning (ML) techniques to understand the reactivities and selectivities of a photochemical cascade reaction towards the first stable polyacetylene, fluoropolyacetylene. I will introduce our new open-access machine learning tool, Python Rapid Artificial Intelligence *Ab Initio* Molecular Dynamics (PyRAI<sup>2</sup>MD), which enables 1,000-fold longer simulations than are currently possible with multiconfigurational NAMD simulations. PyRAI<sup>2</sup>MD has enabled nanosecond ML-NAMD simulations on stereoselective electrocyclic reactions with record degrees of freedom and molecular complexities.

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4:00 PM | CS 24 & Via Zoom