DEPARTMENT OF CHEMISTRY AND ENVIRONMENTAL SCIENCE
SEMINAR SERIES
FALL 2021

DATE: WEDNESDAY, SEPTEMBER 29, 2021

LOCATION: Kupfrian Hall - 117
TIME: 1:00-2:20PM

GUEST SPEAKER

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TOPIC

Quantum chemistry modeling of reactive intermediates with unusual electronic structure

ABSTRACT

Reactive intermediates are high-energy, highly reactive chemical species that typically form stable products after a series of fast chemical transformations. Despite their short lifetimes, reactive intermediates play important role in chemical reactions and are crucial for the rates and product compositions of natural and industrial processes. Recent advances in theory, coupled with the tremendous growth of readily available computational resources, have turned computational chemistry into a powerful tool for studying such intermediates. In certain cases, computational chemistry can provide results on par with the best experimental techniques. Computational chemistry can be used beyond the direct interpretation of the experimental data, as it is capable of discovery of new reaction pathways and novel reactive intermediates. This talk will show several examples of such cases, in which the reactive intermediates are generated using thermal, redox, or light energy. The first part of the talk will focus on the phenomenon of long-bonding in the context of gas-phase photochemistry. The second part will discuss the electronic structure of reactive intermediates generated during the charge transfer through organic materials.

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