UCLA College | Physical Sciences Chemistry & Biochemistry

PHYSICAL CHEMISTRY SEMINAR

Prof. Christine M. Isborn
Chemistry and Chemical Biology
University of California Merced

Monday, Oct. 26, 2020
4:00 PM
via Zoom

“Simulating linear and nonlinear optical spectra for chromophores in the condensed phase”

Accurately modeling molecular excitation and charge transfer has implications that span experimental, engineering, and materials science challenges; for example, the knowledge gained from accurate models would help in interpreting spectroscopic experiments and learning how environmental changes tune electronic absorption and relaxation. Optical spectroscopy is sensitive to the environmental effects but traditional approaches for modeling linear and nonlinear optical spectra of chromophores in complex environments often fail to reproduce spectral shapes due to either lacking vibronic effects and/or missing specific interactions between the molecule and its environment. In this talk I will discuss our new methods for simulating linear and nonlinear optical spectra of condensed phase systems that include vibronic effects and specific interactions with the environment, using both static and dynamic (cumulant-based correlation function) approaches. We will examine the role of quantum mechanical electronic polarization, nuclear quantum effects, anharmonicity, and will showcase a machine learning approach for condensed phase energy gaps to accelerate our spectral calculations.

Please contact marla@chem.ucla.edu for additional information.