CHEMISTRY & BIOCHEMISTRY COLLOQUIUM: Charge Transfer and Interfacial Structure Revealed by Computational Vibrational Spectroscopy

Liang Shi
Assistant Professor, Department of Chemistry and Biochemistry
UC Merced

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Time:
1:30 PM-2:50 PM

Location:
COB 267

About The Speaker:

Liang Shi received his Ph.D. in Chemistry from UW Madison with Prof. James Skinner in 2014. After doing postdoctoral work with Prof. Adam Willard at MIT, he joined UC Merced as an Assistant Professor in 2016. His research focuses on developing and applying multi-scale modeling methods to understand the structure, dynamics, and spectroscopy of complex molecular systems.

Abstract:

Vibrational spectroscopy is a powerful tool to probe the structures and dynamics of condensed phases due to the sensitivity of vibrational modes to the local molecular environment. However, the interplay of many factors in condensed phases, such as structural heterogeneity and charge transfer, can make spectral interpretation challenging, and computational modeling has been helpful in dissecting experimental spectra. In this talk, I will describe two cases where our spectral modeling unveils the underlying molecular structures and dynamics behind the experimental spectra. In the first case, we reproduced the low-frequency infrared (IR) spectrum of liquid water with an improved dipole moment surface using a machine-learning model, and showed that the peak at about 200 cm-1 arises predominantly from the intermolecular charge transfer, instead of polarization. In the second case, our mixed quantum/classical simulation of the IR spectra of the pure phenyl-C61-butyric ac id methyl ester (PCBM) and its blend with poly(3-hexylthiophene) (P3HT) attributed the observed spectral blue shift to the partial orientational ordering of the PCBM side chains at the P3HT/PCBM interface, which has important implications for the exciton dissociation in organic photovoltaics.

For more information, contact : Christine Isborn
cisborn@ucmerced.edu