CHEMISTRY & BIOCHEMISTRY
UCMERCED

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CHEMISTRY & BIOCHEMISTRY SEMINAR SERIES: Probing Reactivity and Interfacial Structure in Water Microdroplets

Abstract:

Aqueous microdroplets have emerged as a promising platform for many chemical syntheses and reactions. Explaining the observed reactivity has proven quite challenging, with many possible mechanisms put forth. Here, I first discuss how the charge of the microdroplets plays a key role in their reactivity. Unlike other possible mechanisms, droplet charge can allow many reactions to occur that are thermodynamically unfavorable in bulk. Next, I discuss our efforts to characterize the structure of the interface, which is also frequently implicated as critical for microdroplet reactivity. We examine a water-hydrophobic interface formed in an oil-in-water emulsion, whose long-term stability and large water-hydrophobic contact area are ideal for characterization. We use Raman-multivariate curve resolution to obtain vibrational spectra of the interface. The spectra differs from that of bulk water, with a decrease in intensity in the lower-frequency parts of the OH-stretch region and the rise of a new shoulder. We develop a novel theory, the monomer field-model, for predicting the Raman spectra directly from molecular dynamics simulations of the interface. By solving the monomer Schrodinger equation, the monomer-field model inherently captures the quantum mechanical couplings relevant for the Raman spectra of liquid water. Our results reveal disorder in the hydrogen-bonding network at the interface, and we assign the new shoulder in the interfacial spectrum to be a “dangling OH” stretch that has been shifted by the presence of a large electric field. This electric field is consistent with the large zeta potential of oil-in-water emulsions has large implications for reactivity at hydrophobic interfaces.

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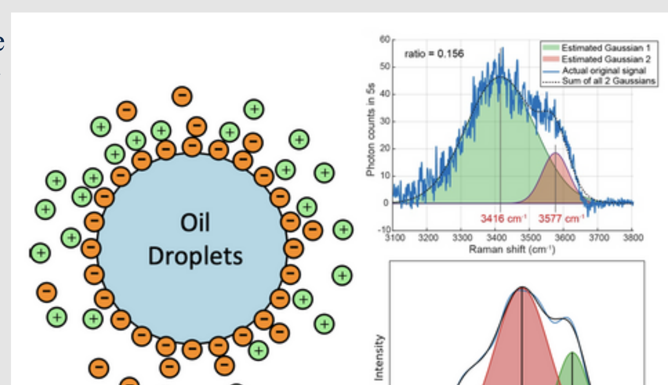

About the Speaker:

R. Allen LaCour is currently a postdoctoral researcher in the Chemical Sciences Division at Lawrence Berkeley National Laboratory. He obtained his BS in chemical engineering at Mississippi State University in 2016. He obtained his PhD in chemical engineering at the University of Michigan, Ann Arbor, in 2022. His current research interests include developing and applying computational spectroscopy methods to characterize molecules in complex environments.

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