

Chem 218: Student Exit Seminar

“Choosing the right lens: Energy surfaces and chemical identity in the photodissociation of Na_2^+ in different solvent environments”

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Abstract: The potential energy surfaces of solution-phase reactions are generally inherited from gas-phase potentials or calculated by assuming that the solvent is in equilibrium with the solute, commonly referred to as the potential of mean force (PMF). However, when the timescale of solvent rearrangement is slower than the motion of the solute, such as some cases of photodissociation, neither the gas-phase surface nor the PMF are expected to accurately describe the energy surface on which the reaction occurs. Using mixed quantum-classical molecular dynamics to simulate the photodissociation of Na_2^+ in liquid Ar and THF, I construct nonequilibrium potential energy surfaces that describe how the presence of solvent molecules affects the reaction dynamics. With Na_2^+ in liquid Ar, solvent caging dominates the dynamics and its effects can be captured using a time-integral of work expression, thereby, reducing a many-body effect onto a single axis. With Na_2^+ in liquid THF, solvent motions are projected onto a structure coordinate that recasts photodissociation as a two-step, sequential process with the first step similar to photoisomerization and the second step as dissociation. This work serves as a foundation for constructing representative solution-phase potential energy surfaces.

**Thursday, March 10th, 2022
12:00 p.m. | Young Hall 2033
& via Zoom**



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