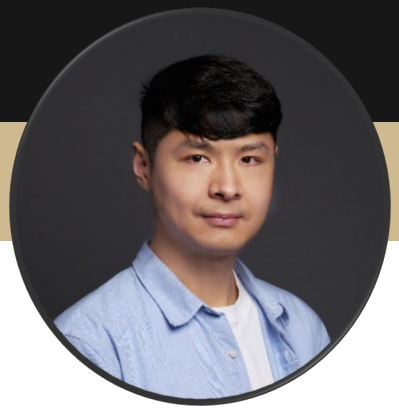

# Physical Chemistry Seminar

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## From Electrons to Ensembles, from Structures to Dynamics: Predictive Chemistry Made Simple

Accurate prediction of chemical mechanisms, structures, and dynamics requires navigating high-dimensional potential- and free-energy landscapes. While ab initio electronic-structure theory can provide the needed accuracy, its computational cost often makes exhaustive exploration impractical, especially when rare events, unexpected pathways, or excited-state processes shape the chemistry. Recent data-intensive pretraining strategies (e.g., neural-network foundation models) offer a promising direction, but high-quality reference data at correlated levels of theory remain difficult to generate at scale, and for photochemistry or dynamical discovery, it is rarely possible to define an adequate training set a priori. In this talk, I will present a physics-driven alternative: pretraining-free surrogate models that adapt on the fly, using occasional ab initio calculations as guidance while maintaining strong physical inductive bias. These real-time surrogate surfaces accelerate structure search, reaction-path optimization, and chemical dynamics, and they provide uncertainty estimates that help decide where new electronic-structure evaluations are most valuable. I will highlight extensions that move beyond ground-state chemistry, including surrogate-driven nonadiabatic photochemical dynamics and highly efficient treatments of nuclear quantum effects. Finally, I will discuss approaches for system–environment interactions, including quantum embedding theory and an electron density-based implicit solvation theory for surfaces and materials, enabling predictive modeling for solution and interfacial reactivity relevant to sustainable chemistry and energy transformation.