Computational Modeling of Enzyme Reactions and Bioimaging Probes

Seminar

Monday

March 2, 2026

3:00 – 4:00 p.m.

Beaupre Center, Room 105

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We will present computational methods from our lab for modeling enzymatic reactions and bioimaging probes. In the first part, we will focus on the identification of the minimum free energy pathway, which is essential to fully understand an enzyme reaction. To reduce the steep computational cost of these free energy simulations, we have adapted the multiple time-step integration algorithm and machine learning potentials in these simulations. We will showcase the power of our simulation protocols with chorismate mutase and CRISPR-Cas9 enzymes. In the second part, we will look briefly at small molecule bioimaging probes. Specifically, we will show how to analyze the interactions between chromophore orbitals and substituent (or solvent) orbitals, and explain how electron-donating and withdrawing groups could modulate the chromophore emission wavelengths.

THE UNIVERSITY OF RHODE ISLAND

Department of Chemistry
Spring 2026 Seminar Series

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