

Steven Boxer Stanford University

Host: Yan Yu



Vibrational Stark Spectroscopy Connects

Electrostatics to Catalytic Rates at Enzyme Active Sites

Electrostatic interactions impact every aspect of the structure and function of proteins, nucleic acids, and membranes. The transition states for many enzyme-catalyzed reactions involve a change in the distribution of charge relative to the starting material and/or products, and the selective stabilization of charge-separated transition states may be essential for catalysis. The magnitudes of the electric fields in proteins and the variations in these fields at different sites are predicted to be enormous, but it is a challenge to obtain quantitative experimental information on these fields. We have developed vibrational Stark effect (VSE) spectroscopy to probe electrostatics and dynamics in organized systems, in particular in proteins where they can report on functionally important electric fields. The strategy involves deploying site-specific vibrational probes whose sensitivity to an electric field is measured in a calibrated external electric field by VSE spectroscopy. This gives the magnitude of the vibrational frequency shift associated with an electric field change in a protein, e.g. by making a mutation, changing pH, ligand binding, etc., projected along the bond axis, which is typically determined by x-ray crystallography.

For further details, contact Mr. Steven Watkins at 5-9749

QCB Seminar Series

Co-hosted by the Department of Chemistry and the Graduate Program in Biochemistry

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C033
2:30 p.m.