Quantum Chemistry
Protein Electric Fields
Enzyme Mechanisms
Molecular Dynamics
Protein Fluorescence
Tryptophan, GFPs, RFPs

REPRESENTATIVE PUBLICATIONS


RESEARCH OVERVIEW

Enzymes enormously accelerate the rates of chemical reactions over the rates of the same reactions in water (by $10^8$-$10^{15}$ fold), but the precise manner by which enzymes accomplish this in detail is still considered an open question.

We are making a seamless transition from obtaining a detailed understanding of how the intense internal electric fields in proteins profoundly affect the properties of tryptophan fluorescence, towards a better understanding and more detailed view of how enzymes attain their astronomical acceleration of biochemical reactions.

We are currently performing classical and quantum molecular dynamics computations on the active sites of many enzymes, with the goal of observing unbiased enzymatic reaction events.