Enzyme Catalysis *in silico*: Using the "Computational Microscope" to Interrogate Reaction Mechanisms and Active Site Structure

Seminar

Friday, November 8, 2024

2:00 – 3:00 p.m.

Beaupre Center, Room 105

With the recent advances in protein structure prediction and cryogenic electron microscopy, computational enzymology is entering a golden age where we can leverage both predicted and experimental structures in studying mechanisms and protein dynamics. In this talk I discuss my work in building experimentally grounded models to demystify how ribonucleotide reductase (RNR) uses long-range proton-coupled electron transfer reactions (PCET) to move a reactive unpaired electron over 32 Å! Particularly, I show how both quantum mechanical and molecular mechanical models of RNR align with the recent structure and experiments, finally allowing us to explain how the environment can modulate the directionality of these PCET reactions. In my postdoctoral work, I discuss how computation has been key to understand how the lack of a bridging ligand in the diiron active site of alkane monooxygenase B impacts its function. Finally, I will preview future research interests in harnessing the millions of predicted protein structures for identification and characterization of proteins that can help us solve pressing environmental issues.

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Fall 2024 Seminar Series

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