Fall 2023 Diversity in Chemistry Symposium

Department of Chemistry and Chemical Biology

Dr. Wendy Shaw

Pacific Northwest National Laboratory

Friday, November 3, 2023

10:00—11:30AM—Panel Session w/ Students
CCB 1209

2:00—3:30PM—Speaker Seminar Presentations
CCB 1303

Host: Professor Kate Waldie

"Inspired By Nature: Understanding Biomineralization Processes and Enzymatic Protein Scaffolds With Advanced Spectroscopy"

Our work focuses on two distinct areas of chemistry: one is understanding how proteins control biomineralization processes, and the second is understanding out the protein scaffold controls catalytic reactivity in enzymes. Our lab brings advanced spectroscopic techniques together to address these very challenging problems. In biomineralization, we are studying amelogenin, a 180 residue protein necessary for proper enamel formation, dictating the resulting intracate crystals which last a lifetime. The mechanistic details of how amelogenin controls crystal growth is not well understood. Protein structure (secondary, tertiary, and quaternary) is thought to play a key role in the function of amelogenin in enamel formation, and the goal of these studies is to understand the structures of the wildtype protein, to allow correlating structure and function in enamel development. We have used solid state NMR, solution state NMR, neutron refliectivity and AFM to develop a molecular level understanding of the protein-surface interface, with broader implications to hard-soft tissue interfaces in tissue repair and replacement. Our catalysis program focuses on trying to capture desirable enzymatic traits in homogeneous catalysts. Dynamics, active site environment and proton channels are the features of the outer coordination sphere that are the focus of these studies. We are developing redox active catalysts which oxidize and produce H_2, mimicking the hydrogenase enzyme. Like other enzymes, hydrogenase enzymes use many outer coordination sphere features to very efficiently convert H^+ to H_2 and back again. Our initial work in this area has focused on incorporating small peptides around the active site of the $Ni(PR_2NR'_2)_2$ hydrogen production/oxidation catalysts to explore how the local environment can influence catalytic rates. More recently we have focused on catalysts for CO_2 reduction. This has resulted in enhanced rates and lowered overpotentials, demonstrating the impact of regions far from the active site. This approach allows us to explore and develop a mechanistic understanding of the role of the outer coordination sphere in both enzymes and molecular catalysts, allowing us to capture the essential features into homogeneous catalysts, with the potential of enhancing the rates, selectivity and specificity of the catalyst.

~Coffee/tea will be served prior to the lecture~

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