CHEMISTRY SEMINAR

Creating and Enhancing a Functional Vanadium Enzyme

By Audrey Moroz ’25 Chemistry

11:30 a.m. **March 30, 2023** **Mara Auditorium**
Masters Hall Rm 110

Abstract:

Vanadium, an abundant metal in nature, is often not used in biological settings, due to its uncontrolled hydrolysis. However, by utilizing the *de novo* Due Ferri single-chain (DFsc) protein system, which has two iron binding sites and was modeled to mimic natural proteins, we aim to build vanadium enzymes. Because the catalytic applications of vanadium have been a widely studied topic of research, we looked to expand the catalytic activity of vanadium. In nature, these enzymes often function as haloperoxidases. Although vanadium is a hydrolysis-prone metal, these haloperoxidases are able to carry out their reactivity in water, something that has not been reproduced by any lab-designed mimic. The active site of the native DFsc protein was modified to include a series of arginine residues to better mimic the vanadium haloperoxidase active sites that are known to utilize vanadium. Using colorimetric assays, the activity of these vanadium-bound species have been measured to determine their ability to function as haloperoxidases. To better characterize this system, we have also utilized cyclic voltammetry to monitor the effect that an increasing number of arginine residues has on the redox potential of the bound vanadium, where we have seen shifts based on protein identity.

CHEMISTRY SEMINAR

Modeling Water-soluble Chlorophyll Binding Protein with Quantum Mechanics/Molecular Mechanics Simulation

By Henry Namiot ’23 Chemistry

11:30 a.m. **March 30, 2023** **Darrah Auditorium**
McCreary Hall Room 101

Abstract:

Water-soluble Chlorophyll-binding proteins (WSCPs) are pigment-protein complexes that are not directly involved in photosynthesis. However, due to their simple structure they have served as a valuable model in studying other photosynthetic pigment-proteins. This paper provides results using ORCA and NAMD to investigate different properties of Chlorophyll and WSCP. Using ORCA, absorption spectra were predicted using different functionals. They were found to be self-consistent but did not agree with experimental results in the larger wavelength range. This paper has also used the results of hybrid quantum mechanical/molecular mechanical (QM/MM) molecular dynamics (MD) simulations completed using NAMD. Time dependent density functional tight binding (TD-DFTB) contained in the DFTB+ software package was used to compute the electronic excitations of each of the Chlorophylls contained in the class IIb WSCPs. Site energies of the individual chlorophylls, excitonic couplings, spectral densities, and reorganization energies are reported. All results agree closely with experimental results. Additionally, the high frequency range of the spectral density was found to demonstrate exceptional quantitative agreement in comparison to previous QM/MM MD works. We observe in our results an exhibition of the homo-tetrameric structure of the WSCP. We also observe a minimization of the “geometry mismatch” problem.