

Understand the Chemistry and Photophysics of Vitamin B2 Derivatives Through Computational Multiscale Models

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ABSTRACT: Flavins (vitamin B2 derivatives) are organic cofactors bound by around 1-3% of known proteins. Their diverse chemical roles as electron and proton/hydrogen/hydride acceptors makes them highly versatile organic molecules capable of catalyzing a wide range of chemical reactions. Flavins are also blue-light absorbing chromophores, a property harnessed by almost all living organisms for various light-sensing functions, such as in LOV, BLUF, and CRY, and for light-driven catalysis, such as in DNA repair. These properties of flavins have been capitalized on by researchers to develop artificial flavoproteins for biotechnological and medical applications including bioimaging, biosensing, photodynamic therapy, (photo)catalysis, and optogenetics. However, engineering new functions can be done much more efficiently by first understanding, at the molecular level, how these proteins work. Spectroscopy is among the most powerful tools available to study the chemistry of flavoproteins. An alternative tool, growing rapidly in popularity over the past few decades, is computational modeling, which is the area of our research: we apply hybrid quantum mechanical and molecular mechanical models to aid in the interpretation of flavoprotein spectroscopy and to model excited-state processes. In my talk, I will discuss our recent efforts to develop and apply multiscale computational models to simulate the UV/visible spectroscopy, fluorescence, infrared spectroscopy, photophysics, and redox potentials of flavin-binding proteins.

References

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