Design of (Bacterio)chlorophyll Inspired Antenna Systems for Artificial Light-harvesting Devices

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Renewable energy sources, particularly solar energy, are crucial to supply mankind's increasing demands. In this regard, artificial photosynthesis represents a promising research area where natural photosystems can be employed as models for designing and engineering synthetic light-harvesting devices. For instance, the Light-harvesting system 2 (LH2) and its constituting Bacteriochlorophyll (BChl) chromophores represent a great example of studying Nature's way of collecting and channeling solar energy. Understanding the mechanisms and the fine details regulating energy absorption and transfer in LH2 represents a major challenge.
Within this research topic, in the presented project, we employ advanced computational chemistry tools to accurately describe the photochemical properties of novel, BChl-inspired, chromophore models, aiming to assess their spectroscopic characteristics.
Moreover, the multichromophoric aggregates of natural and synthetic light-sensitive complexes absorb light at different wavelengths compared to their constituent molecules. Thus, the assessment of the underlying intermolecular interactions (i.e., couplings) is crucial when trying to understand and rationalize the behavior of such systems. Consequently, we evaluate the aggregate behavior for numerous dimeric derivatives of BChl-like systems thanks to a recently developed code, integrated into the OpenMolcas Program [1][2], that allows for the assessment of the inter-monomeric couplings, in the spirit of Frenkel Exciton Hamiltonian model.
The implemented computational methods enable an accurate description (at the multireference, multiconfigurational level of theory) of the photochemical and photophysical properties of the pigment units and set the basis for the future development of novel artificial photosynthetic devices.

1. Kaiser et al. (2023) J Chem Theory Comput 19, 10, 2918-2928
2. Li Manni et al. (2023) J Chem Theory Comput 19, 20, 6933–6991