Multiscale modeling of light harvesting and energy transfer in photosynthesis

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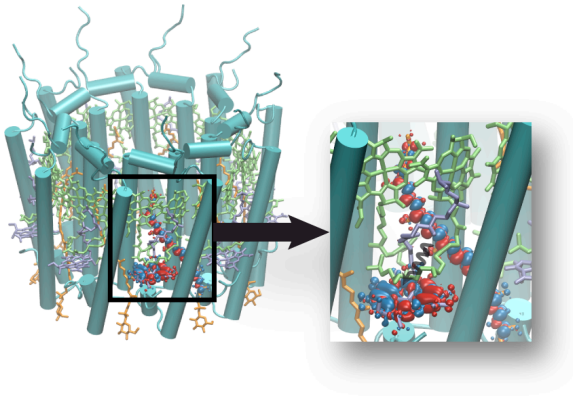
The environment plays an important role in the light harvesting dynamics of photosynthetic pigment-protein complexes.[1] Specific pigment-protein interactions modulate the energy levels of the pigments, thus defining the spatial pathways of energy transfer. On the other hand, the polarizable properties of the environment screen electronic couplings between pigments, a key quantity that determines exciton delocalization and migration dynamics. Moreover, coherent energy transfer recently observed in several photosynthetic complexes has been suggested to arise from the structured-nature of the spectral density that quantifies the coupling of electronic excitations to the vibrations in the system.



Here we overview a combined QM/MM-MD strategy we have developed that allows exploring the impact of the environment in full atomic detail on site energies, electronic couplings and spectral densities, accounting for mutual polarization effects among the chromophores and their environment through polarizable force fields.[1,2] We discuss the main insights unveiled by this strategy by investigating the properties of several pigment-protein complexes, including phycobiliproteins from cryptophyte algae, the Fenna-Matthews-Olson (FMO) complex of green sulfur bacteria and the water-soluble chlorophyll binding protein (WSCP) of higher plants.

1. C. Curutchet, B. Mennucci, *Chem. Rev.* **117** 294–343 (2017).
2. C. Curutchet et al., *J. Am. Chem. Soc.* **133** 3078–3084 (2011).