Principles of Solar Energy Conversion in Photosynthesis

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Life on Earth relies on the ability of photosynthetic organisms to utilize sunlight for generating electron transfer cascades and proton gradients. These power redox reactions that include water oxidation and CO_2 fixation. The initial conversion of excitation energy, i.e. of sunlight captured by pigments, into the electron flow that drives all subsequent redox chemistry takes the form of super-fast and perfectly efficient charge separation at “reaction centers”, special assemblies of strongly coupled protein-embedded tetrapyrrole pigments such as chlorophylls. How reaction centers achieve this feat remained fundamentally unknown until recent advances in modelling their electronic structure. Here I discuss how computational chemistry provides unprecedented insights into the primary processes of photosynthesis by combining multiscale/multilevel simulations of membrane-embedded proteins with quantum chemical methods that describe excited states of pigment assemblies. Our research shows that the ability to separate charge and to transfer electrons with specific directionality emerge solely from protein matrix electrostatics. Matrix anisotropy strongly differentiates otherwise chemically identical pigments, enabling them to perform novel collective functions. These results shift the focus from the pigment to its environment as the key for understanding the molecular principles of solar energy conversion and for interpreting spectroscopy and electron transfer kinetics, while also suggesting a distinct biomimetic design concept for artificial photosynthesis.