How Photosynthesis Works: Insights from Multiscale Simulations

Dimitrios A. Pantazis
Max Planck Institute for Coal Research, Mülheim an der Ruhr, Germany

Life relies almost entirely on the ability of photosynthetic organisms to utilize sunlight for powering the synthesis of complex chemicals. Photosystem II (PSII) is the enzyme responsible for the initial conversion of excitation energy into the flow of electrons that sustains subsequent redox processes, as well as for catalysing the all-important oxidation of water into dioxygen. Primary charge separation takes place at the reaction centre of PSII, a special assembly of strongly coupled pigments, while water oxidation is catalysed by a manganese-containing multinuclear metallocofactor that is unique in biology, the oxygen-evolving complex (OEC). The detailed electronic structure description of both the reaction centre and the OEC cluster are essential for achieving an atomic-level understanding of their function. This requires multiscale/multilevel simulations that incorporate classical and quantum chemical methods able to tackle the structural complexity of the system, account for protein electrostatics, perform reliably for excited states of pigment assemblies, and connect with complex experimental data obtained by optical and magnetic resonance spectroscopies. Here I discuss advances in our understanding of the molecular mechanisms of oxygenic photosynthesis, describing how multiscale simulations offer fundamental insights into the electronic structure and properties of individual photosynthetic components, but also uncover the crucial role of the protein matrix in enabling primary charge separation and in facilitating the delicate atomic choreography embodied in the catalytic cycle of water oxidation.