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Protein matrix control of photosynthetic processes: insights from multiscale simulations

Oxygenic photosynthesis is responsible for sustaining the biosphere of our planet. The unique membrane protein complex Photosystem II (PS-II) is the cornerstone of this process, using sunlight to drive a series of complex and intertwined redox transformations that result in generation of oxygen and eventually enable CO_2 fixation. Crucial components of its function include charge separation among embedded chlorin pigments and the all-important 4-electron catalytic oxidation of water into dioxygen by the manganese-containing cluster of the oxygen-evolving complex. Reliable correlations between geometric/electronic structure and experimental observations are essential for elucidating the principles governing the function of PS-II. Here I will describe the efforts of our research group to understand selected aspects of the function of PS-II using a variety of computational methods that cover different scales of simulation, from molecular mechanics and dynamics to the most recent implementations of correlated wave function theory. A particular point of focus will be the role of the protein matrix, which has only recently begun to be clarified. Among others, I will discuss how the protein is responsible for regulating access to the catalytic site of water oxidation and how protein matrix electrostatics are responsible for regulating the remarkable photochemistry that takes place in the reaction center of PS-II.