Charge transport in the D2 branch of Photosystem II and Electrical conductance of DNA and RNA

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Photosynthesis, the fundamental process sustaining life on Earth, depends on the Photosystem II (PSII) reaction center's ability to initiate the charge transport process. Using multi-scale simulation methodologies, we have investigated this charge transport process with a focus on the dissimilarity between the two branches of the PSII reaction center, D1 and D2. Utilizing Marcus theory, we have calculated the reorganization energies and activation barriers for all the key steps involved in the charge transport process. Our analysis reveals that while both D1 and D2 branches exhibit similarities in the initial stages, the rate-determining step in the D2 branch has a significantly higher activation barrier (0.2 eV) than D1 branch (0.1 eV), suggesting a much less favorable energetic landscape. Further, the calculation of current-voltage (I-V) characteristics confirms the higher resistance in the D2 branch compared to the D1 branch, emphasizing its non-conductive nature. If time permits, we will also report the electrical conductance of native DNA and RNA and in the presence of oxidatively damaged basses. Oxidatively damaged DNA can act as molecular diodes with a record tunable rectification ratio of as high as 10^6.

References:

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