Hydrophobic mismatch model for cytochrome b_6f driven state transitions is attractive for computer simulations

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In contrast to the bacterial anoxygenic photosynthetic membranes, which have one photosystem (PS) and cytochrome bc_1 complex (cyt bc_1), the oxygenic photosynthetic membranes have PSII and PSI, and cyt b_6f between them. Both cyt b_6f and bc_1 perform proton-coupled electron transfer, but cyt b_6f also triggers the short-term regulatory mechanism of oxygenic photosynthesis state transitions. State transitions balance the distribution of the excitation light energy between PSII and PSI via light-harvesting complexes redistribution. However, a molecular mechanism for cyt b_6f driven state transitions is not yet evidenced. Recently, we revealed the role of the single chlorophyll a (Chl*a*) molecule in cyt b_6f by parallel analysis of numerous X-ray crystal structures of cyt b_6f and bc_1. We found correlations between the Chla molecular volume and cyt b_6f X-ray crystal structures changes and proposed a completed new molecular mechanism for cyt b_6f driven state transitions that has no analog in other biological membranes [1]. On the other side, our studies on the kinetics of state transitions in a variety of field plants pointed out to possible evolution-assisted changes in the amino acid sequence of cyt b_6f. With this presentation we would like to attract the attention of the biomathematical community to the hydrophobic mismatch model for induction and progression of membrane structural reorganizations. We will show why the molecular dynamics simulations would be beneficial to evidence the hydrophobic mismatch model.

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[1] Vladkova, R.; Chlorophyll a is the crucial redox sensor and trans-membrane signal transmitter in the cytochrome b_6f complex. Components and mechanisms of state transitions from the hydrophobic mismatch viewpoint. Journal of Biomolecular Structure and Dynamics, 34:4(2016) 824-854.