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LECTURE

"The Photosynthetic Apparatus under Stress by Molecular Simulations"

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Scientists are constantly targeting the life-sustaining oxygen cycle that is driven by the processes of photosynthesis and cellular respiration. Especially the insight into the dynamics of the photosynthetic apparatus (Photosystem II, PSII) has applications in the artificial solar energy harvesting, or the increase of crop yields. Light Harvesting Complexes (LHCII) of PSII absorb the solar energy and transfer excitons to be utilized at the reaction centres (RC), via an elaborate network of chlorophyll pigments. There is however a drawback in this natural process under excess (or fluctuating) light conditions: a photoprotective mechanism is activated to convert a significant amount of exciton energy into heat, and to protect against RC damages. The mechanism is called Non-Photochemical (Chlorophyll Fluorescence) Quenching, or NPQ. NPQ protects the apparatus against overloading, it is triggered by an excess ΔpH across the thylakoid membranes and by the interaction of LHCII with the PSII subunit S (PsbS). In this talk, the focus will be on large-scale Molecular Simulations that reveal a pathway that starts with the induction of ΔpH and the LHCII-PsbS interaction and continues with the perturbations on the elaborate pigment network that formulate the quenching sites, where excess energy is dissipated as heat.