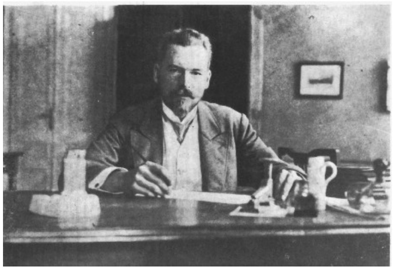

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The versatile role of plastic crystals in light harvesting

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One route towards capturing solar energy with great efficiency is to fundamentally investigate the way nature is capable of performing the different stages in photo-synthesis. Chlorosomes - large antennae complexes found in Green Sulfur Bacteria - are unique in capturing and transporting photon energy with near 100% quantum efficiency to the reaction centre where electrons and holes are separated for downstream usage. An interesting feature is that these huge antennae are able to perform an important biological function in the absence of regulatory proteins. Being composed of pigments only, chlorosomes offer a possibility for studying how light harvesting is encoded in the plastic-crystalline phase behavior and particularly in its dynamic disorder, and why the coupling between electronic, atomistic and molecular degrees of freedom gives rise to such great efficiency. Earlier, we performed systematic large-scale molecular dynamics (MD) simulations of chlorosomes in order to resolve the unknown pigment packing and the dynamic disorder within it. Next, we coupled this structure to a Frenkel Hamiltonian for calculating the exciton evolution and study the role of dynamic disorder in fast excitation energy transfer (EET), a mechanism that remains unresolved up to date. We found that the dynamic disorder, as encoded in a varying Frenkel Hamiltonian, has the effect of localising coherent domains, but that it at the same time accelerates transport of excitonic energy over the assembly structure via an enhanced mixing of overlapping eigenstates of very similar energy. In this presentation, we provide the details of this intriguing mechanism.

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