Optical signals of photosynthetic antenna complexes modulated by microsecond protein dynamics

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The plant antenna complex light-harvesting complex II (LHCII) is a key player in natural photosynthesis. LHCII occurs as a trimeric protein complex and contains 42 chlorophylls. Its chromophores are responsible for capturing photons and transmitting the excitation energy towards the photosystem II reaction center. This challenging task requires a highly precise chromophore arrangement resulting in a specifically fine-tuned ordering of the energy levels and couplings.
We built a coarse-grained (CG) model of LHCII using the Martini force field which allows us to study the LHCII dynamics in the thylakoid membrane on a hundreds of microseconds time scale (Fig. 1a) [1]. Using tools from machine learning, we extracted the most prominent structures (Fig. 1b) via a density-based clustering algorithm. The chlorophyll arrangements of these structures are used to calculate the electronic couplings between the chlorophylls by means of the extended dipole model. Based thereon, we use an excitonic Hamiltonian to simulate linear absorption, circular dichroism (Fig. 1c), and two-dimensional electronic spectra.

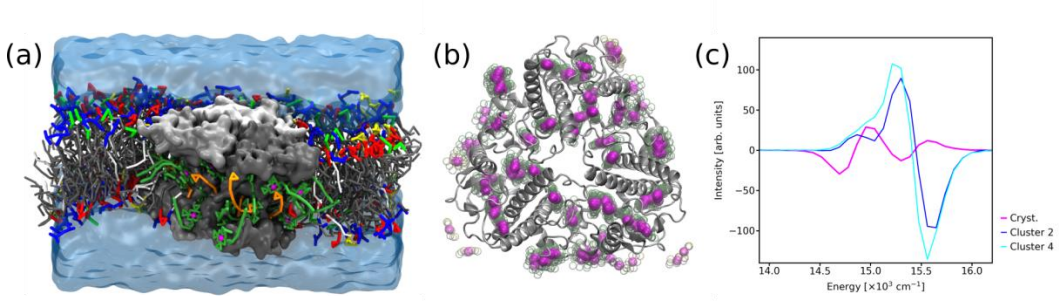

Figure 1: Simulation box containing a LHCII trimer in thylakoid membrane (a), extracted clusters from a 10 µs CG MD trajectory (b), circular dichroism spectra for the two most prominent clusters and the crystal structure (c).

Our study shows that the sampled configurations of trimeric LHCII span a manifold of chromophore arrangements. Moreover, these individual arrangements have a pronounced impact on the optical properties of LHCII trimers. We will discuss the impact of the microsecond protein dynamics on the electronic spectra of LHCII and to which extent the protein matrix dynamics results in an increased diversity of excitonic conditions for the excitation energy transfer.

References

1. S. Thallmair, P. A. Vainikka, and S. J. Marrink, *Biophys. J.* **116** (2019), 1446.