Large scale simulations of photosynthetic antenna systems: interplay of cooperativity and disorder

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Abstract

Large scale simulations of light-matter interaction in natural photosynthetic antenna complexes containing more than one hundred thousands chlorophyll molecules, comparable with natural size, have been performed. Photosynthetic antenna complexes present in Green sulfur bacteria and Purple bacteria have been analyzed using a radiative non-Hermitian Hamiltonian, well known in the field of quantum optics, instead of the widely used dipole-dipole Frenkel Hamiltonian. This approach allows to study ensembles of emitters beyond the small volume limit (system size much smaller than the absorbed wavelength), where the Frenkel Hamiltonian fails. When analyzed on a large scale, such structures display superradiant states much brighter then their single components. An analysis of the robustness to static disorder and dynamical (thermal) noise, shows that exciton coherence in the whole photosynthetic complex is larger than the coherence found in its parts. This provides evidence that the photosynthetic complex as a whole has a predominant role in sustaining coherences in the system even at room temperature. Our results allow a better understanding of natural photosynthetic antennae and could drive experiments to verify how the response to the electromagnetic
radiation depends on the size of the photosynthetic antenna.

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