Challenges for theoretical modelling - excitons in porphyrin nanotubes

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Self-assembled tubular aggregates, such as those formed by the TPPS4 porphyrin (see Fig. 1), are a class of materials mimicking the structure of the photosynthetic antenna complexes of green bacteria (the chlorosomes). They exhibit unique linear and non-linear optical properties, as well as effective excitation energy transport, and therefore are of a fundamental interest as a model system to study the nature and dynamics of excitons in molecular assemblies of reduced dimensionality and for understanding the photophysical processes occurring in natural light harvesting systems. Furthermore, potential applications in optoelectronic, energy transport and light harvesting make them attractive from the practical perspective.

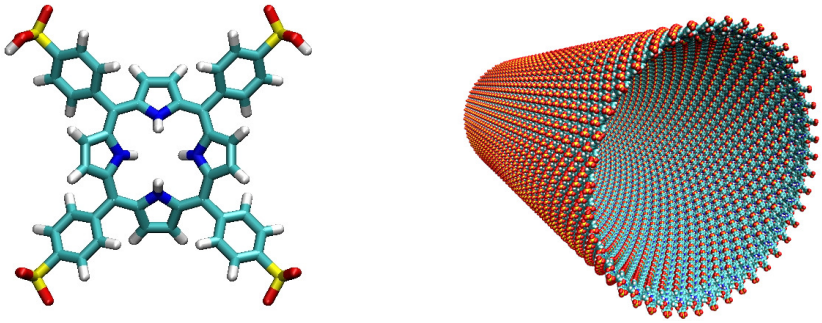

Figure 1- Structure of the monomer and the aggregate of TPPS4.

However, the complex interplay of various interactions combined with a large number of molecules within the aggregate makes theoretical modelling of excited states and their optical dynamics in systems such as TPPS4 nanotubes a challenging task. We combine several methods to take into account all the relevant interactions: intermolecular resonance interactions, intermediate strength exciton-phonon coupling, as well as the effects of static and dynamic disorder. We model linear absorption and dichroism as well as the pump-probe spectra of TPPS4 nanotubes. The good agreement with the experimental data opens up the perspective for studies of the exciton diffusion.