A computational study of structural and excitonic properties of chlorosomes

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Propositions

belonging to the thesis entitled

A Computational Study of Structural and Excitonic Properties of Chlorosomes

1. Chlorosomes form stable tubular matrices carrying robust dynamic structural disorder, which can be traced back to the twisting frustration of their *syn-anti* packing units.
   Chapter 2 and 3, this Thesis

2. Chlorosomes and other tubular molecular aggregates exhibit unique optical spectra depending on their chirality or chiral angle; this can be clarified using computational methods.
   Chapter 3 and 5, this Thesis

3. Dynamic disorder in the electronic coupling, *i.e.* the off-diagonal terms in the excitonic Hamiltonian, plays a vital role in the high efficient excitonic energy transfer process in chlorosomes.
   Chapter 3 and 4, this Thesis

4. Tails of BChl pigments in different layers of tubular chlorosomes do not interdigitate with each other; they play a vital role in the stability, assembly kinetics, and mechanical properties of chlorosomes.
   Chapter 2 and 6, this Thesis

5. The chlorosome is a masterpiece of molecular designing that happens in nature.

Bryant, D. A.; Canniffe, D. P., J. Phys. B: At., Mol. Opt. Phys. ***2018****, 51, 033001*

6. To understand the excitonic energy transfer in chlorosomes, it is better to starts from an eigenstate of the exciton Hamiltonian instead of a state fully localized on a single site.
   Chenu, A.; Maly, P.; Mancal, T. Chem. Phys. ***2014****, 439, 100–110*

7. It is possible to generate large tubular molecular aggregates as convenient as generating carbon nanotubes, see the generator (CTubeGen) for chlorosomes developed in this thesis.
   This Thesis and DOI:10.5281/zenodo.3677027

8. The helical structure of chlorosome carries two vital features enhancing their light-harvesting capacity: spacing saving and enlarged conformational entropy.
   This Thesis and Snir, Y.; Kamien, D. R. Science ***2005****, 307, 1067*

9. Data visualization helps in computational studies, even for optical entertainment purposes.

10. Being immersed in a research project long enough, one may find that insight from daily life starts to help.

11. "*il meglio é nemico del bene*" (an Italian proverb means "perfect is the enemy of good"); this is especially true for the simulationers.

12. If there is a hole, there is a hole.