

Spectral manifestation of C_2 modulation of the LH2 complex of Purple bacteria

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C_2 modulation in the B850 rings was suggested from single-molecule studies. It can manifest in various forms; five of which are discriminated based on single-molecule, linear and two-dimensional spectroscopy. We find that a model with C_2 modulated diagonal disorder fits best with all the experimental results.

Investigating the processes in the natural light harvesting systems not only promote understanding of photosynthesis, it can also serve as potential solution to our energy need through integrating with the solar technology. Since the chromophores used by purple bacteria as the light-harvesting complex is structurally much simpler than the corresponding system in plants, purple bacteria is a tractable choice for the studies. Previous spectroscopic studies on light harvesting 2 (LH2) complex have suggested presence of C_2 modulation in its B850 ring [1]. We investigated the manifestation of such modulation on the two-dimensional spectra and found that it is suitable to discriminate among various models. One model is put forward that agree reasonably well all the experimental spectroscopic results. Still the physics behind these modulations is not understood on an atomistic level.

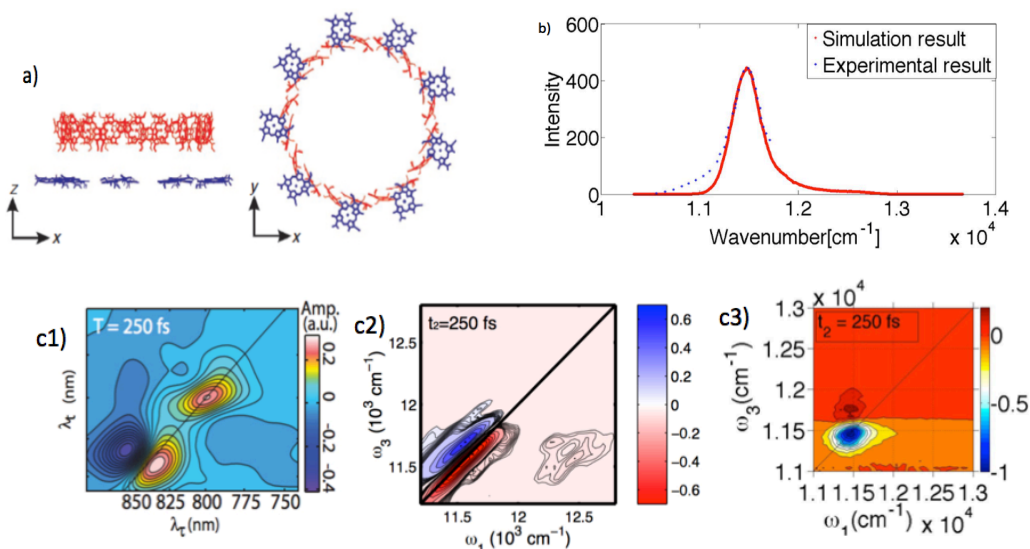


Fig 1: a) Geometrical arrangement of the BChl molecules of the LH2 complex of RPS. *Acidophila*. Blue one depicts the B800 ring and red one depicts the B850 ring¹. b) Simulated linear absorption spectrum with experimental result² considering C_2 modulation in the ring. c1) Experimental two-dimensional spectrum³. c2) Calculated two-dimensional spectra for a model with varying radii of B850 rings⁴. c3) Calculated two-dimensional spectra for a model with C_2 modulation in the B850 ring. All presented two-dimensional spectra are for 250 fs waiting times.

¹ A. M. van Oijen et al., *Science* 285, 400 (1999)

² S. Georgakopoulou et al., *Biophys. J.* 82, 2184 (2002)

³ A. F. Fidler et al., *J. Chem. Phys.* 139, 155101 (2013)

⁴ C. P. van der Vegte et al., *J. Phys. Chem. B* 119, 1302 (2015)