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Modelling Excitonic Energy Transfers in *Bryopsis corticulans* using 2D Electronic Spectroscopy

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Abstract

We apply a phenomenological fitting method to the two-dimensional electronic spectra of the light-harvesting complex II (LHCII) from *Bryopsis corticulans* (*B. corticulans*) at 77 K to extract information about the excitonic states and energy transfer processes. *B. corticulans* is a marine green alga whose photosynthesis adapts to the underwater environment; thus, its properties are expected to deviate from the widely studied plant LHCII to some extent. The fitting method results in well converged parameters, including eight excitonic energy levels with their respective transition dipole moments, spectral widths, energy transfer rates and coupling properties. The 2D spectra simulated from the fitted parameters concur very well with the experimental data, proving the robustness of the fitting method. An excitonic energy transfer scheme can be constructed from the fitting parameters, which is described for the first-time for *B. corticulans* LHCII. The strength of our phenomenological fitting method in obtaining excitonic energy levels and energy transfer network is put to good test in systems such as *B. corticulans* LHCII where prior knowledge and exact assignment and spatial locations of pigments are lacking. We hope future full structural determination of *B. corticulans* LHCII can validate our predictions.

Keywords: Photosynthesis; Light harvesting complexes; Excitonic energy transfer; Modelling; Two dimensional optical spectroscopy.