New Simulations of 2D spectra of Photosystem II Reaction Center

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Two dimensional spectra of photosystem II reaction center are simulated and compared with experimental results. Significant improvement comparing with previous simulations is achieved, by using a more suitable theoretical approach and updated model parameters.

Two dimensional spectroscopy (2D) has recently contributed new insights to energy and charge transfer, and coherent dynamics in the photosystem II reaction center (PSIIRC) [1-3]. Analysis of kinetics in the 2D spectra provided information about the timescales of excited state dynamics [1], while coherence analysis have shown that charge transfer might be stimulated by vibrational degrees of freedom [2,3]. Previous simulations of the 2D spectra of PSIIRC achieved qualitative agreement with experimental data [4], however, they were constrained by the theoretical approach used. Indeed, the application of the modified Redfield theory to describe the spectral lineshapes could lead to deviations from accurate results [5].

Here we extend and apply the approach suggested in [5] to the 2D spectra calculations, and use the new theory for simulation of 2D spectra of PSIIRC. Our results show considerable improvement if compared to previous work (Fig. 1).

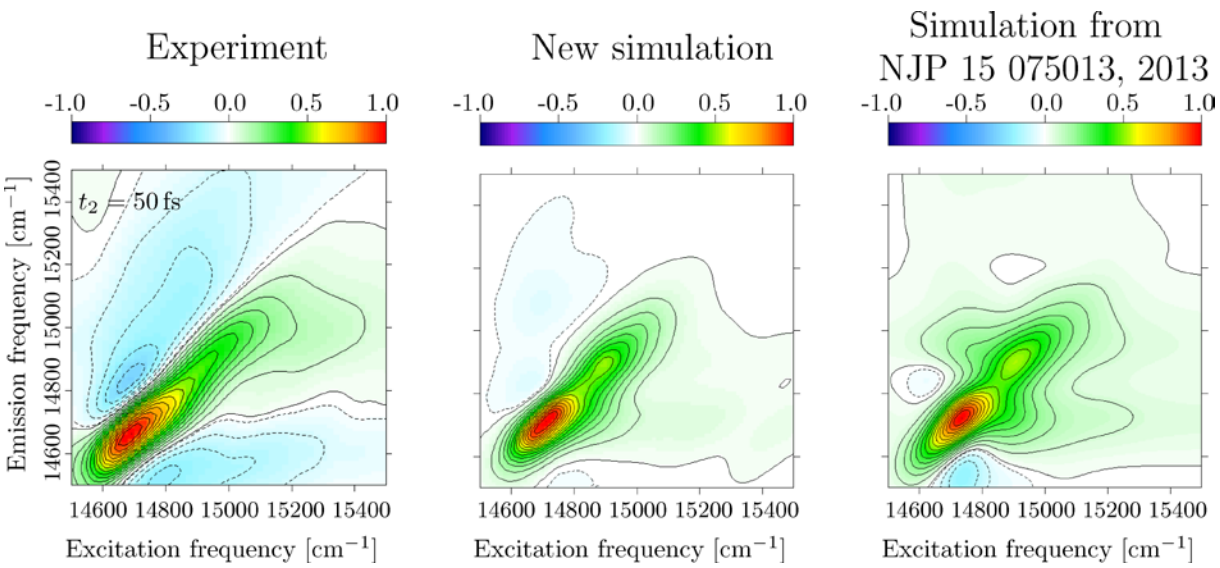

Fig.1 Comparison of experimental 2D spectra of PSIIRC with simulated results.

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