Towards a Quantum Dynamical Model of Charge Separation in the Photosystem II Reaction Center

Thorsten Hansen[1,*] and Lea N. Sørensen[1]

[1]*Department of Chemistry, University of Copenhagen, Copenhagen, Denmark*
**thorsten@chem.ku.dk*

Sunlight absorbed by green plants induces charge separation in the reaction centers of photosystems I and II. In the summer of 2014, two spectacular papers demonstrated 2D electronic spectra of the photoinduced dynamics in the photosystem II reaction center[1,2]. The past decade has brought extensive new experimental data. Detailed theoretical understanding is still outstanding.

In this work, we build a quantum dynamical model for the reaction center. Key parameters are calculated with computational chemistry[3]. Subsequently, the 2DES spectra are simulated using Redfield dynamics. First generation of our modeling is restricted to exciton dynamics and may be good for a few hundred femtoseconds. We present our current model and looks ahead.

References

[1] F.D. Fuller *et al*., *Nature Chemistry*, 2014, **6**, 706.
[2] E. Romero *et al*., *Nature Physics*, 2014, **10**, 676.
[3] L.N. Sørensen *et al.*, *ACS Omega*, 2024, .