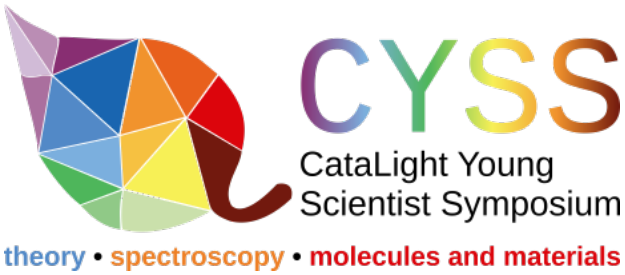

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Transient Absorption 2D Correlation Spectroscopy – A Kinetic Model Free Approach to the Analysis of Ultrafast Spectroscopy Data

Thursday, 30 September 2021 10:40 (20 minutes)

Time-resolved femtosecond transient absorption (fs-TA) spectroscopy is a powerful method to investigate the photoinduced processes in molecular systems, that is, their relaxation and reaction pathways upon photoexcitation on time scales between a few femtoseconds and hundreds of nanoseconds. Analysis of the resulting set of spectra generally requires advanced techniques which try to fit a kinetic model to the data, for example via global lifetime analysis or multivariate curve resolution. While these methods are widely used, they require a priori information on the sampled system, as they require a kinetic model, i.e., the number of processes contributing to the data. Choosing the right number of processes is often not an easy task and heavily influences the results.¹

2D correlation spectroscopy (2DCOS), a method popular especially in the field of vibrational spectroscopy, offers a way to analyze systematic changes in datasets recorded under a changing external variable, by recovering the cross-correlation function of the spectral variables.² 2DCOS is ideally suited to TA spectroscopy, as the external variable (time) is inherent to the method. Furthermore, it does not require a specific kinetic model or other a priori information. TA-2DCOS allows the extraction of the number of kinetic processes contributing to the data set alongside qualitative spectral signatures. We demonstrate that TA-2DCOS can reproduce the results obtained by common, model dependent, methods for well understood systems. 2DCOS can therefore serve as an alternative analysis method for fs-TA spectra and offer an ideal starting point for quantitative methods, if a priori information is not available.³

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