Charge transfer in mixed valence states: relaxation dynamics and transient absorption spectroscopy

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Quantum dynamical model calculations are performed on the photo-induced electron transfer in a mixed valence system interacting with different solvents. The simultaneously occuring processes of non-adiabatic population transfer and relaxation are studied in detail. Transient absorption traces, as recently recorded in our laboratory [1], are simulated, and the features of the spectra are related to the dynamics. The agreement with experiment hints at the fact that the employed one-dimensional models catch the essentials of the photochemistry of the investigated systems, and that it can be used for the interpretation of the transient-absorption spectra. It is inferred that the ultrafast electron-transfer processes take place on a sub-picosecond time scale and afterwards relaxation occurs within several picoseconds.

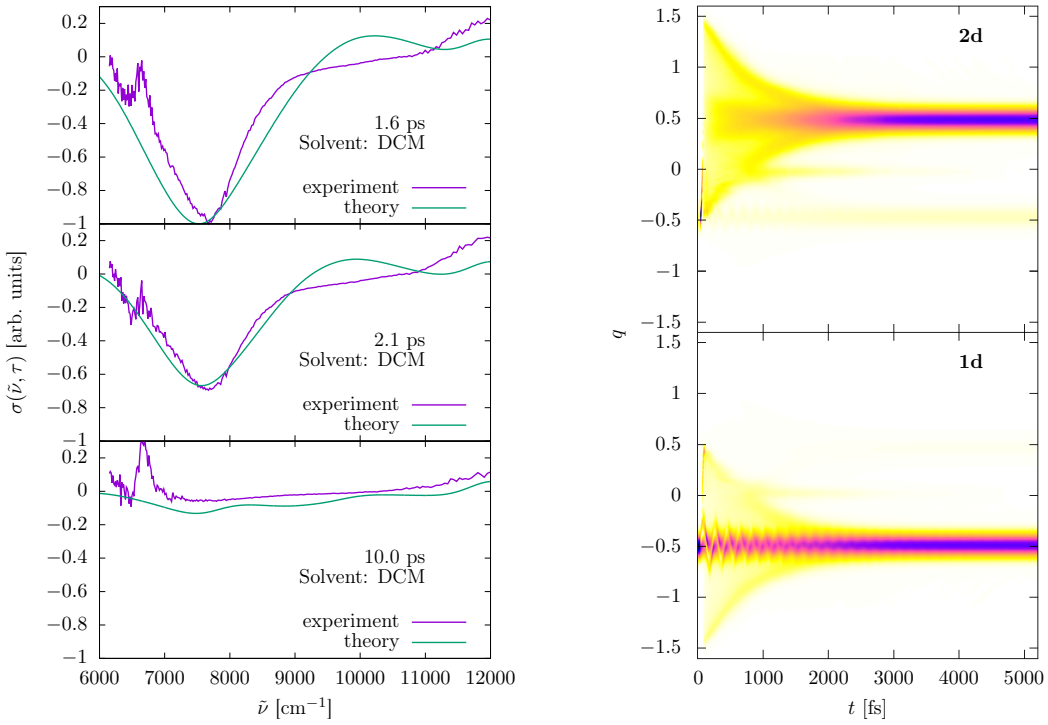

Figure 1: Comparison of measured and calculated spectra (left) and the wave-packet dynamics in the two diabatic states (1d, 2d) after laser excitation (right). Initially, only the 1d-state is populated.

References

1. Lambert et al., *Phys. Chem. Chem. Phys.* **18**, (2016), 19405