AKjDPG 2: Tutorial Molecular Spectroscopy (joint session AKjDPG/MO)

Time: Sunday 16:00–18:00 Location: U HS 224

Tutorial AKjDPG 2.1 Sun 16:00 U HS 224

How Ultrafast Spectroscopy Can Follow Molecular Reaction Dynamics in Real Time — •Patrick Nuernberger — Physikalische Chemie II, Ruhr-Universität Bochum, 44780 Bochum

Physicists and chemists are usually very familiar with absorption spectrometers. The obtained spectra provide information on energy levels and further properties of the substance at hand. Whereas one directly determines which photon is absorbed and how well, some of the most interesting information is not accessible in this way: what happens directly *after* the photon has interacted with the molecules?

Quite intuitively, one needs to measure at a later time to find out. Instead of looking only at the reaction's start and finish, a comprehensive approach has to follow the dynamics in real time in order to identify intermediates and decipher the underlying reaction mechanisms. For this, laser pulses in the femtosecond range are required, since photophysical processes and photochemical reactions (where bonds are cleaved and formed) may occur on an ultrafast time scale.

In this tutorial, the basics of ultrafast molecular spectroscopy are introduced. Different experimental implementations and the applicability to systems ranging from diatomic molecules to large biosystems are discussed. Two versatile approaches, transient absorption and coherent two-dimensional spectroscopy, are analyzed in detail with illustrative examples.

Tutorial AKjDPG 2.2 Sun 17:00 U HS 224

Theoretical Perspective on Time-resolved Spectroscopy of Molecular Systems — •Oliver Kühn — University of Rostock, Institute of Physics, 18059 Rostock, Germany

Experiments in ultrafast spectroscopy have advanced to an unprecedented level of sophistication, being able to unravel even the finest details of molecular dynamics. Applications range from gas phase dynamics to the initial steps of photosynthesis, thereby encompassing many orders of magnitude as far as time and frequency scales are concerned. The analysis and interpretation requires advanced theoretical methods that can cope with the challenges provided by the experimental data. Here, ideas from electronic structure theory and quantum dynamics meet, areas which evolved separately so far.

In this tutorial, basic concepts of theoretical time-resolved spectroscopy will be discussed using applications from recent literature. In particular it will be shown that in the weak-field limit a rigorous and practical formulation of (non-)linear signals in terms of multi-time response functions can be given. Their information content is fully explored within two-dimensional spectroscopies, which have been developed to probe vibrational as well as electronic excitation dynamics.

[1] V. May and O. Kühn, Charge and Energy Transfer Dynamics in Molecular Systems, Wiley-VCH, 2011; [2] P. Hamm and M. T. Zanni, Concepts and Methods of 2D Infrared Spectroscopy, Cambridge, 2011; [3] M. Schröter, S. D. Ivanov, J. Schulze, S. P. Polyutov, Y. Yan, T. Pullerits, O. Kühn, Phys. Rep. 567, 1 (2015).