PHYSIKALISCHES KOLLOQUIUM

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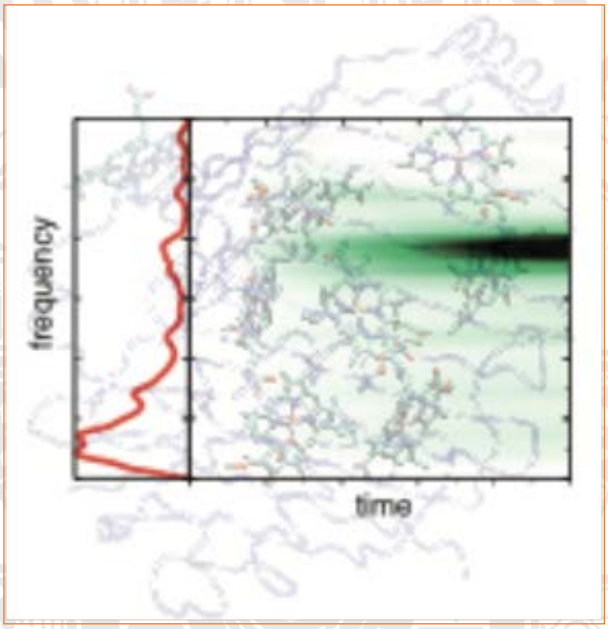
IM GROßEN HÖRSAAL



DYNAMICS AND SPECTROSCOPY OF FRENKEL EXCITONS IN NATURAL AND ARTIFICIAL LIGHT-HARVESTING

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Excitation energy transfer in supramolecular architectures covers a broad range of dynamical regimes, depending on the electronic properties of the constituent dye building blocks, their mutual Coulomb interaction, as well as the coupling to vibrational degrees of freedom and to some solvent or protein environment. Following the discovery of long-lived coherent oscillations in the FMO light- harvesting complex by means of two-dimensional spectroscopy considerable attention has been paid to the role of exciton-vibrational coupling, which goes beyond that of a mere heat bath for disposing excess energy. Fortunately, with the development multilayer multilayer multiconfiguration time-dependent Hartree approach, a theoretical tool is available to address such dynamics in great detail. However, a prerequisite is the spectral density describing the exciton-vibrational coupling beyond simple models.

This presentation will focus on the spectroscopy and quantum dynamics of artificial molecular aggregates and crystals as well as the photosynthetic FMO complex. It includes the discussion of a new protocol for the calculation of spectral densities based on the self-consistent charge, tight-binding DFT method as well as high-dimensional quantum dynamics simulations for FMO complex using an experimental spectral density.