Advanced Atomic and Molecular Physics

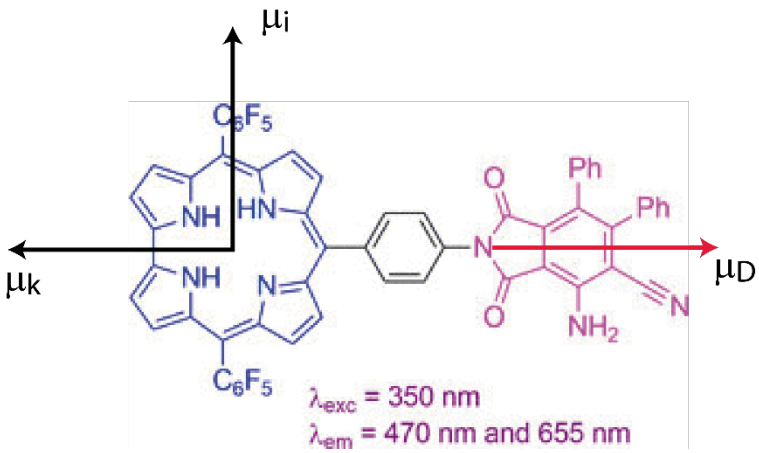
Prof. Heyne

2017-07-05
Bonus

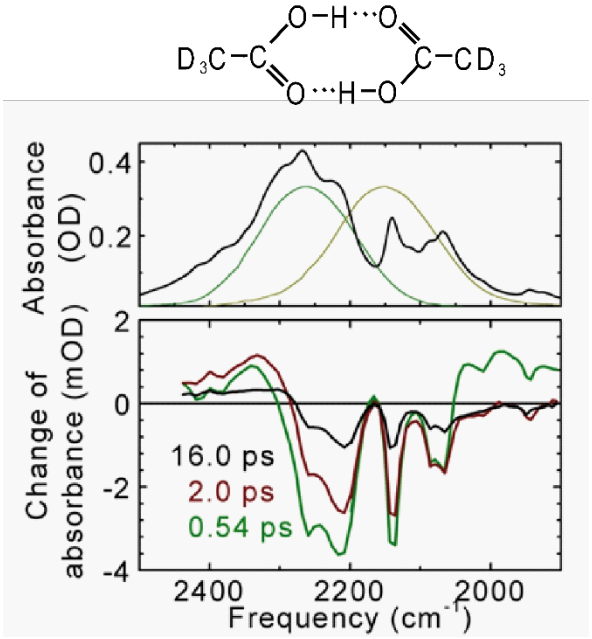
10. assignment

Deadline: lecture Thursday (2017-07-13)

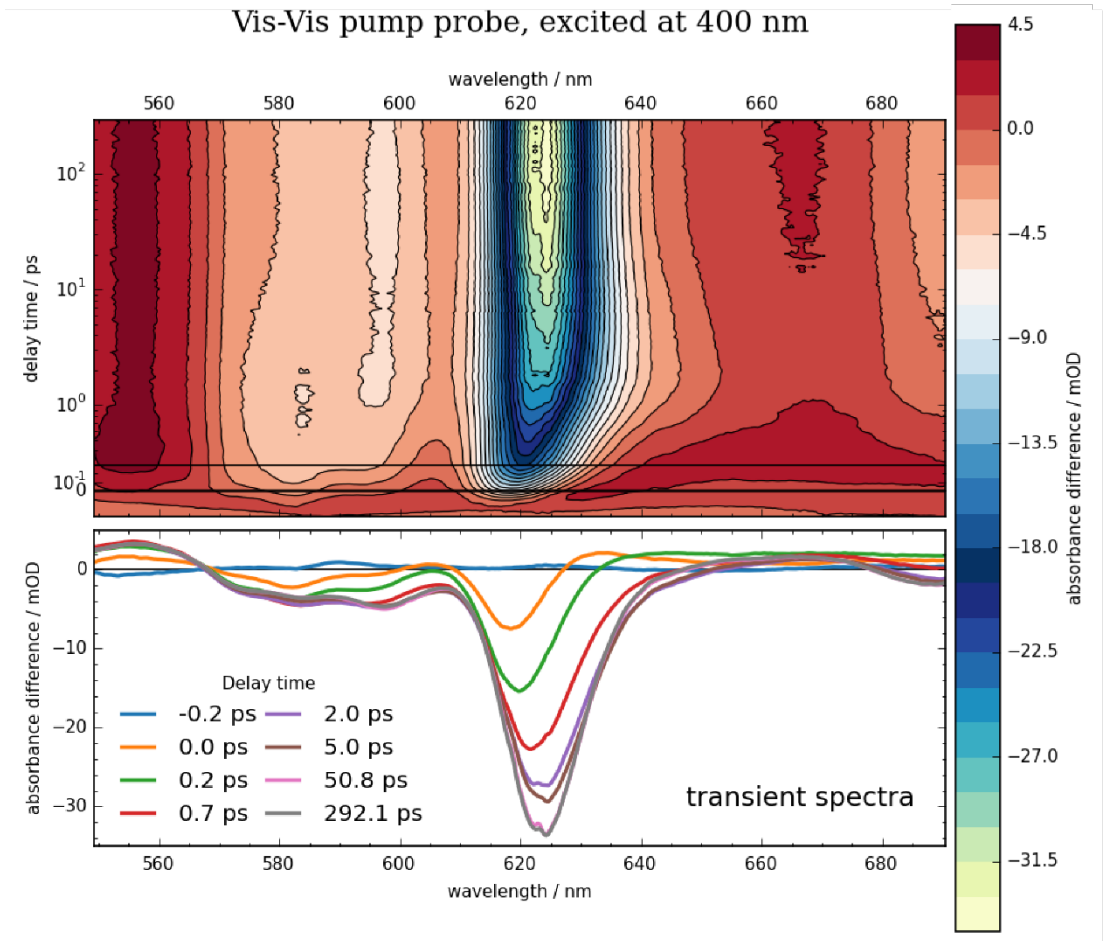
1.) (2 points) Calculate the dipole-dipole interaction V between μ_i and μ_D, as well as between μ_k and μ_D. Calculate with a distance R of 11 Å.



2.) (4 points) In the figure below transient IR pump – IR probe data of deuterated acetic acid dimer are presented. The Gaussian curves represent the intensity profile of the pump pulses. The excited vibrations are the hydrogen bonded O-D stretching vibrations of deuterated acetic acid dimers. Identify the positive and negative signals and sketch the transitions in a level diagram. Note, the OD-stretching vibration has a decay time of a few hundreds of femtoseconds. After relaxation, the excess energy of the IR pump pulse is distributed over the molecule resulting in excitation of low-frequency modes that weakens the hydrogen bond.



3.) (5 points) In the figure below a contour plot of VIS pump – VIS probe data of Al(tpfc)(py)$_2$ (upper panel) and a selection of transient absorbance difference spectra (lower panel) are shown. Negative signals indicate an increase of signal at the detector



(negative absorption signals), while positive signals indicate a loss of signal at the detector (positive absorption signals). The linear absorption spectrum (violet line) and fluorescence spectrum (red line) were presented in the 9. assignment. The absorbance differences are depicted as a function of pump-probe delay time and probe wavelength. Identify the positive (excited state absorption) and negative signals (bleaching signal, stimulated emission). Sketch the dynamics in a Jablonski diagram. Identify the dynamics and estimate the time scale of the dynamics visible in the measured time window. The excitation at 400 nm promotes the system to a higher excited electronic state (S_3 or S_4). Note, the time scale from -200 fs to 200 fs is blurred by nonlinear artefacts.