MO 58: Poster: Molecular Dynamics (Theory)

Zeit: Donnerstag 16:30–18:30 Raum: Poster A

MO 58.1 Do 16:30 Poster A

On the geometry dependence of molecular dimer spectra with an application to aggregates of perylene bisimide — •Joachim Seibt[1], Philipp Marquetand[1], Zhijian Chen[2], Volker Dehm[2], Frank Würthner[2], and Volker Engel[1] — [1]Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Institut für Organische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

We study spectroscopic properties of molecular dimers coupled by dipole-dipole interactions within the framework of time-dependent quantum mechanics. A systematic variation of the dimer geometry allows to establish relationships between the latter and structures in the absorption spectrum. The theoretical model is constructed with the purpose to characterize the changes in absorption and emission properties arising upon aggregation of perylene bisimides. Measured and calculated spectra are compared, thereby addressing the question if a simple exciton model is capable to describe excited state properties of nanoaggregates of these molecules [1].

[1]J. Seibt, P. Marquetand, V. Engel, Z. Chen, V. Dehm, F. Würthner, Chem. Phys. 328, 354 (2006).

MO 58.2 Do 16:30 Poster A

Decoherence of vibrational wave packets — •Martin Schlesinger and Walter Strunz — Theoretische Quantendynamik, Physikalisches Institut, Universität Freiburg, Hermann-Herder-Str. 3, 79104 Freiburg

We clarify the effect of rovibrational coupling on the coherence of molecular vibrations [1]. Depending on the temperature chosen we observe a significant suppression of (fractional) revivals in the pump-probe signal [2]. As a measure of coherence we calculate the purity of the vibronic density operator and find a remarkable oscillatory behaviour on the vibrational time scale. Finally we extend our investigations to dimers attached to He nanodroplets [3].

[1] T. Baumert, V. Engel *et. al.*, Chem. Phys. Lett. **191**, 6 (1992)
[2] C. Brif, H. Rabitz *et. al.*, Phys. Rev. A **63**, 063404 (2001)
[3] P. Claas, G. Droppelmann *et. al.*, J. Phys. B (submitted)