

Dienstag, 15.10.2013

Hörsaal D, Chemiezentralgebäude, 17:15 Uhr

Sprecher: **Andreas Untereiner**
(Universität Karlsruhe)

Titel: **Ultrafast relaxation dynamics of
molecules in solution**

Abstract:

Energy dissipation of molecules in solution is of utmost importance in many different areas of science. In this contribution we will first focus on the elucidation of energy pathways of metalloporphyrins.¹ - 4 Femtosecond pump-probe absorption spectroscopy as well as transient anisotropy was used to follow the dynamics of the corresponding Mg-, Zn- and Cd-compounds in tetrahydrofuran as main solvent. These studies were accompanied by (time-dependent) density functional calculations. Based on experimental findings and calculations, a model for the relaxation pathway of these systems is presented. Thereby, the existence and energetics of so-called dark states (one-photon forbidden transitions from the electronic ground state) will be discussed as well as the competition between internal conversion and intersystem crossing. The latter issue becomes even more important when considering another system, monomeric molecules for photoinduced polymerization that have been studied with ultrafast spectroscopy techniques, too⁵ and thus, first results will be presented.

¹ O. Schalk, H. Brands, T.S. Balaban, A.-N. Unterreiner, *J. Phys. Chem. A* (2008), 112, 1719.

² Y. Liang, M. Bradler, M. Klinger, O. Schalk, M. C. Balaban, T. S. Balaban, E. Riedle, A.-N. Unterreiner, *ChemPlusChem* (2013), DOI: 10.1002/cplu.201300143.

³ Y. Liang, O. Schalk, A.-N. Unterreiner, *EPJ Web of Conferences* (2013), 41, 05014.

⁴ O. Schalk, Y. Liang, A.-N. Unterreiner, *Z. Phys. Chem.* 227 (2013), 35.

⁵ T. J. A. Wolf, D. Voll, C. Barner-Kowollik, A.-N. Unterreiner, *Macromolecules* (2012), 45, 2257.

Organisation: P. Nürnberger