CPP 20 Dynamics II

Zeit: Dienstag 11:15–12:30 Raum: TU C230

CPP 20.1 Di 11:15 TU C230

Single molecule fluorescence experiments on homo polymers and block copolymers. — •Heiko Zettl, Ute Lippert, Wolfgang Häfner, Alexander Böker, and Georg Krausch — Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth

In recent years single molecule methods like fluorescence correlation spectroscopy and single molecule tracking became increasingly important for the study of the (bio) macromolecules. Here, we present single molecule experiments on dye labelled synthetic polymer chains in organic solvents and in thin polymer films. We aim at studying the dynamics of single polymer chains in complex polymeric environments. Fluorescence correlation spectroscopy was used to determine the hydrodynamic behaviour of single polymer chains in dilute and semi-dilute polymer solutions. To extent the experiments towards longer time scales, single molecule tracking was used to follow the motion of single chains in a microphase separated polymer matrix.

CPP 20.2 Di 11:30 TU C230

Charge and Energy Dynamics in Photo-Excited poly(para-phenylenevinylene) Systems — •Linus Gisslén[1,2], Sven Stafström[2], and Åsa Johansson[2] — [1]Institut für Physik, Technische Universität Chemnitz, Chemnitz, Germany — [2]Department of Physics and Measurement Technology, Linköping, Sweden

We report results from simulations of charge and energy dynamics in poly(para-phenylenevinylene) (PPV) and PPV interacting with C_{60}. The simulations were performed by solving the time-dependent Schrödinger equation and the lattice equation of motion simultaneously and nonadiabatically. The electronic system and the coupling of the electrons to the lattice were described by an extended three-dimensional version of the Su-Schrieffer-Heeger model, which also included an external electric field. Electron and lattice dynamics following electronic excitation at different energies have been simulated. The effect of additional lattice energy was also included in the simulations. Our result show that both exciton diffusion and transition from high to lower lying excitation are stimulated by increasing the lattice energy. Also field induced charge separation occurs faster if the lattice energy is increased. This separation process is highly nonadiabatic and involves a significant rearrangement of the electron distribution. In the case of PPV coupled to C_{60}, we observe a spontaneous charge separation. The separation time is in this case limited by the local concentration of C_{60} molecules close to the PPV chain.

CPP 20.3 Di 11:45 TU C230

NMR Investigations of Adsorbed Molecules in Zeolites — •Özlen Ferruh Erdem and Dieter Michel — Institut für Experimentelle Physik II, Universität Leipzig, Linnéstrasse 5, D-04103 Leipzig, Deutschland

High-resolution ^{1}H MAS and ^{2}H NMR spectroscopy are used to study the behaviour of ethylene glycol adsorbed in NaX zeolites. Typical changes in the proton chemical shift values for the CH_2 and OH groups arise which are very sensitive to interactions between the molecules and the internal surfaces. This allows to clearly differentiate between molecules within the zeolite cages and those ones adsorbed at the outer surface of the zeolite grains as well as to study the dynamics of the different species. Selective measurements of the proton longitudinal relaxation times T_1 were carried out for both type of the molecules which show large differences in the thermal mobility when the pore filling degree is varied. For molecules inside the supercages, a dynamic heterogeneity occurs. This may be related to the competing influences of molecule-molecule interactions within the network of intermolecular hydrogen bonds and molecule-surface interactions. ^{2}H NMR measurements are performed for deuterated ethylene glycol adsorbed in NaX for the characterisation of the phase transition from liquid-like to glass-like behaviour.

CPP 20.4 Di 12:00 TU C230

The Perylene TiO_2 System: Analysis of a Heterogeneous Electron Transfer Reacation — •Luxia Wang[1], Ralph Ernstorfer[2], Frank Willig[2], and Volkhard May[1] — [1]Institut für physik, Humboldt Universität zu Berlin, Newtonstraβe 15, D-12489 Berlin — [2]Hahn-Meitner-Institut, Abteilung Dynamik von Genzflächenreaktionen Glienicher Str. 100, 14109 Berlin

To understand details of heterogeneous electron transfer reactions is of huge importance for the development of photo–voltaic devices. We report on recent experimental as well as theoretical results on photoinduced ultrafast charge injection from perylene into empty (conduction band like) states of TiO_2 nanocrystals. Concentrating on the influence of different anchor groups which fix the dye at the TiO_2 surface a consistent understanding of cw–absorption spectra as well as of femtosecond transient absorption could be achieved [1]. The rather unique model obtained in this way is used to suggest femtosecond laser pulse control of the charge injection process [2].

[1] L. Wang, R. Ernstorfer, F. Willig, and V. May, J. Phys. Chem. B (in press).

[2] L. Wang and V. May, J. Chem. Phys. **121**, 8039 (2004).

CPP 20.5 Di 12:15 TU C230

Organic monolayers for UV-pump/XUV-probe measurements of molecular dissociation — Peter Siffalovic[1], •Martin Michelswirth[1], Frank Hamelmann[1], Peter Bartz[1], Björn Decker[2], Olaf Batron[2], Thorsten Meyer[3], Manfred Neumann[3], Jochen Mattay[2], Ulrich Heinzmann[1], and Markus Drescher[1] — [1]Molekül und Oberflächenphysik, Fakultät für Physik, Universität Bielefeld — [2]Organische Chemie I, Fakultät für Chemie, Universität Bielefeld — [3]Elektronenspektroskopie, Fachbereich Physik, Universität Osnabrück

Self-assembled Calixarene-molecules on flat substrates are promising templates for dynamical studies of guest-host-interaction. Attached iodine atoms are removed by selectively breaking bonds with femtosecond UV (266 nm) pulses. The evolution of the iodine dissociation can be followed with time-resolved ESCA utilising femtosecond XUV (13 nm) pulses. Signal quality and temporal resolution depend on an effective control of detrimental effects from multiphoton electron emission. To this end different substrate materials are tested.