CPP 23: Electronic and Optical Properties

Time: Wednesday 14:00–17:00 Location: ZEU 114

CPP 23.1 Wed 14:00 ZEU 114

Analyzing Anisotropic Light Propagation by Defocused Imaging of Single Emitters — •Rebecca Wagner and Frank Cichos — Molecular Nanophotonics Group, University of Leipzig, Linnéstraße 5, 04103 Leipzig

Many materials introduce an optical anisotropy to internal emitters due to their internal structure. Layers of oriented polymer molecules have different dielectric constants parallel and perpendicular to the layer, i.e. they are birefringent. Photonic crystals, materials with periodic variation of the dielectric constant, have stop bands for certain directions in which propagation of light is prohibited. These effects have been measured for example by angle resolved fluorescence spectroscopy for ensembles of emitters, thereby averaging over extended areas. However, if the anisotropy is caused by the local environment of the emitters, a spatially-resolved measurement is necessary. We show that optical anisotropy can be measured locally by defocused imaging microscopy of internal emitters. This leads to asymmetric diffraction patterns that contain information about the spatial dependence of the emission. We show how these patterns are influenced by the angle dependence of the refractive index ellipsoid. The technique is demonstrated exemplarily on photonic crystals to measure the fractional local density of states, i.e. the angle dependence of the photonic stop band.

CPP 23.2 Wed 14:15 ZEU 114

2d light point locallisation in stretchable planar waveguide — •Anton Neulinger[1,2], Petr Bartu[1], Robert Koeppe[1,2], Lisa Fallon[3], Nikita Arnold[1], and Siegfried Bauer[1] — [1]Department of Soft Matter Physics (SoMaP), JKU Linz, Altenbergerstr. 69, A-4040 Linz, Austria — [2]isiQiri interface technologies GmbH i.G., c/o tech2b, Hafenstr. 47-51, A-4020 Linz, Austria — [3]Dublin Institute for Advanced studies (DIAS), 31 Fitzwilliam Place, Dublin 2, Ireland

A fully flexible and stretchable planar waveguide serving as a photoluminescent concentrator, fabricated from a mixture of PDMS with a fluorescence dye, can be used to detect localized light. The incident light is absorbed by the dye, leading to an emission of light with higher wavelength. The emitted light is spreading out in the two dimensional waveguide and detected via embedded Si-photodiodes in the device. Using a simple mathematical model, the position of light spots can then be easily recalculated. These devices can lead to applications, such as human interface devices and artificial skins. This work was partially supported by FWF.

CPP 23.3 Wed 14:30 ZEU 114

Infrared Transition Moment Orientational Analysis (IR - TMOA) — •Periklis Papadopoulos, Wilhelm Kossack, and Friedrich Kremer — Universität Leipzig, Institut für Experimentelle Physik I, Linnéstr. 5, 04103 Leipzig

A novel method is suggested for unraveling the mean orientation and the molecular order parameter in any IR-transparent or translucent material under study. It is based on the analysis of IR transmission spectra as a function of polarization and an intentional inclination of the sample. Taking advantage of the specificity of the IR spectral range, it is based on the analysis of the absorption coefficient $\alpha \sim \left\langle \left(\vec{\mu} \cdot \vec{E}\right)^2 \right\rangle$, where mu is the transition dipole moment and E the electric field of the IR beam, in dependence on the polarization and the angle of inclination. Additionally, for non-scattering samples, the complex refractive index tensor can be determined by using the Fresnel equations. The spatial resolution of the technique is only limited by the wavelength.

Compared to other structural techniques, like X-ray scattering and NMR, this novel method has the advantage that it can give group-specific 3D structural information for samples under varying external conditions. The sample quantity requirements are minimal (down to μg) and time-resolved studies in combination with mechanical or electric measurements may be carried out.

CPP 23.4 Wed 14:45 ZEU 114

Coplanar waveguides - new sample cells for fast and ultrafast investigations — •Michael Görlich[1,2,3,4], Klaus Attenkofer[1], Nalaka Kodituwakku[1], Manfred Fickenscher[2], Reinhard Foijt[3], and Ignaz Eisele[4] — [1]Argonne National Laboratory — [2]Hochschule München — [3]Ketek GmbH — [4]Universität der Bundeswehr München

Motivated by the idea of using coplanar waveguides (CPW) as a sample cell to trigger and control chemical reactions, the infrastructure for designing, testing, and simulating these transmission lines was developed. Unlike any other method CPWs offer the opportunity to create extreme high field strengths of up to 1V/nm in combination with an excitation length of pico- and sub-picoseconds. A fundamental understanding and characterization of CPWs in different frequency ranges was obtained and theoretical limits to field strength and frequency were derived. A test facility was designed, built, and commissioned to characterize the electric properties of transmission lines built in integrated circuit technology. The important part of the measurements and results will be presented.

CPP 23.5 Wed 15:00 ZEU 114

Oscillator strength of the peptide bond resonances at the C 1*s* and N 1*s* X-ray absorption thresholds — •Kurt Kummer[1], Victor Sivkov[2], Denis Vyalikh[1], Serguei Nekipelov[2], Anja Blüher[3], Michael Mertig[3], and Serguei Molodtsov[1] — [1]Institute of Solid State Physics, Dresden University of Technology, D-01062 Dresden, Germany — [2]Komi Science Center, Russian Academy of Science, Ural Division, Syktyvkar 167982, Russia — [3]BioNanotechnology and Structure Formation Group, Max Bergmann Center of Biomaterials and Institute of Materials Science, Technische Universität Dresden, D-01062 Dresden, Germany

X-ray absorption of regularly arrayed two-dimensional bacterial surface layers of *bacillus sphaericus NCTC 9602* was investigated by means of total electron yield measurements. In doing so the spectral dependence of the total absorption cross section in the photon energy range between 280 and 580 eV was obtained, as well as partial absorption cross sections at the C 1*s*, N 1*s* and O 1*s* edges. At each of the three edges a sharp resonance originating in the peptide group showed up. For the very first time, the oscillator strengths of C $1s \rightarrow \pi^*$(CONH) and the N $1s \rightarrow \pi^*$(CONH) transitions were determined. Furthermore, we demonstrate that the folded structure of the protein leads to an increased oscillator strength of incorporated benzene rings when compared to free benzene molecules.

15 min. break

CPP 23.6 Wed 15:30 ZEU 114

New thiol-gold binding protocol for improving the conductance of double-stranded DNA — •Shoupeng Liu[1], Benjamin Bornemann[2], Andreas Marx[2], Elke Scheer[2], and Artur Erbe[1] — [1]Physics Department, University of Konstanz, D-78457 Konstanz, Germany — [2]Chemistry Department, University of Konstanz, D-78457 Konstanz, Germany

Thiol-functionality at 5' ends DNA are normally used to allow its binding to gold electrodes for measuring its conductance. However, poor overlap of the electronic orbitals of the thiols with the Pi-system leads to low conductance of DNA. In this contribution, new oligonucleotides are synthesized that bear short thioalkyl functions at the nucleobases rather than at the phosphor-sugar backbone. We investigated the electronic transport properties of double-stranded DNA ended with these new oligonucleotides by mechanically controllable break junctions (MCBJ). From the measured current-voltage characteristics we deduce a semiconductor-like electronic band-structure. The results suggest a comparatively high conductance with a current of 700 nA in 0.25V, which is higher than in most of the former reports. The improved conductance is suggested to be caused by the thioalkyl group which facilitates charge transfer into the Pi-system of the nucleobases.

CPP 23.7 Wed 15:45 ZEU 114

Advanced Simulation Methods for Charge Transport in OLEDs — •Evelyne Huber, Hansueli Schwarzenbach, Roger Häusermann, Nils A. Reinke, and Beat Ruhstaller — Zurich University of Applied Science, Institute of Computational Physics, Wildbachstrasse 21, 8401 Winterthur, Switzerland

Until now the system of equations for organic semiconductor device modelling has been predominantly solved in a decoupled way with the

Gummel algorithm which can suffer from slow convergence. This limits the use of fitting algorithms for parameter extraction and sweeping. For the design of OLED it is of crucial importance to solve the involved equations efficiently on a PC. OLED simulation requires solving the continuity equations for electrons and holes and the Poisson equation in one dimension. The resulting system of equations is strongly coupled. Introducing disorder and novel mobility models for organic materials leads to highly nonlinear equations. In this study we present OLED simulations where the coupled equations are solved with the Newton algorithm. We combine this method with advanced physical transport models such as Gaussian disorder, density- and field-dependent mobilities and generalized Einstein diffusion. The performance of the presented algorithms is compared.

CPP 23.8 Wed 16:00 ZEU 114

Angular electronic "band structure"of molecules — •Yaroslav Pavlyukh and Jamal Berakdar — Martin-Luther-Universität Halle-Wittenberg

First principles calculations of the electronic structure of spherical molecules reveals that the valence band dispersion and bands filling are almost completely determined by the properties of angular momentum operator. With a very high accuracy we find the single particle states to disperse with the averaged angular momentum ℓ as $E_\ell = E_0 + \ell(\ell+1)/2R^2$. Angular electronic band bendings at large ℓ and all peculiarities in the band fillings of large fullerenes and their high symmetry derivatives can be explained within a unified picture as bands avoided crossing.

CPP 23.9 Wed 16:15 ZEU 114

Laser-excitation of molecular systems within stochastic time-dependent current-density-functional theory — •Heiko Appel and Massimiliano Di Ventra — Department of Physics, University of California, San Diego, USA

In this talk we investigate the excited electron dynamics of molecular systems due to laser excitation. The system dynamics is described within the recently proposed stochastic time-dependent current-density-functional theory [1,2]. Work supported in part by Lockheed Martin and DOE.

[1] Massimiliano Di Ventra and Roberto D'Agosta, Phys. Rev. Lett. **98**, 226403 (2007).
[2] Roberto D'Agosta and Massimiliano Di Ventra, Phys. Rev. B **78**, 165105 (2008).

CPP 23.10 Wed 16:30 ZEU 114

Three-Pulse Photon Echo beyond the Impulsive Limit — •Ines Mynttinen[1], Wichard J. D. Beenken[1], Tönu Pullerits[2], and Erich Runge[1] — [1]Technische Universität Ilmenau, Germany — [2]Lund University, Sweden

We present computational simulations of three-pulse photon echo (3PPE) experiments on Nile-blue as a reference. For the theoretical analysis, we go beyond the impulsive limit in order to simulate the effects of duration and chirp of the incoming laser pulses. In particular, we study the time-integrated intensity of the third order polarization, the frequency-resolved polarization, and the photon-echo peak shift. The latter is defined as the value of the first delay time where the maximum integrated signal intensity occurs for given second delay time. The peak shift is of general importance for the use of 3PPE in condensed-matter studies, since the time evolution of the peak shift was found earlier to reflect the time-correlation function of the system-bath interaction. We found that both, finite pulse duration and chirp, result in a distinct decay of the integrated intensity in dependence on the second delay time. Additionally, the chirp affects the decay of the peak shift. Our results make clear that it is necessary to control the chirp of the pulses in 3PPE experiments. In particular, the frequency-resolved third-order polarization signal allows to distinguish between the fundamental system-bath dynamics and the effects caused by the pulse chirp. Furthermore, careful analysis of the chirp dependence proves to be a tool to extract additional information from 3PPE experiments, which is usually hidden due to the finite pulse duration.

CPP 23.11 Wed 16:45 ZEU 114

Effect of chemical architecture on light-induced deformation in azobenzene polymer films — •Marina Saphiannikova[1], Vladimir Toshchevikov[1,2], and Gert Heinrich[1] — [1]Leibniz-Institut für Polymerforschung, Dresden, Germany — [2]Institute of Macromolecular Compounds, Saint-Petersburg, Russia

Photoresponsive azobenzene polymers have been extensively explored as highly functional materials which have a fascinating potential for technical applications (data storage media, artificial muscles, etc). We propose a microscopic theory which describes the light-induced deformations in amorphous azobenzene polymers taking the chemical architecture of macromolecules explicitly into account. Our theory provides the values of the light-induced stress comparable and higher than the values of yield stress typical for glassy polymers. Thus, the theory explains the possibility for the inscription of surface relief gratings in glassy azobenzene polymers in the absence of light-induced softening. We show that the photo-elastic behaviour of azobenzene polymers is very sensitive to the chemical architecture. Depending on the chemical architecture, a sample can be either stretched or uniaxially compressed along the electric vector of the linearly polarized light. For some chemical architectures, elongation of a sample displays a non-monotonic behaviour with the light intensity. These predictions are in agreement with experimental observations [1] and MD simulations [2].

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[1] D.Bublitz et al. Appl. Phys. B 2000, 70, 863
[2] J.Ilnytskyi et al. MCLC 2008, 496, 186