CPP 11: Poster: New Instruments and Methods

Time: Monday 16:30–18:00 Location: Poster C

CPP 11.1 Mon 16:30 Poster C

Versatile Object-oriented Toolkit for Coarse-graining Applications — Victor Rühle, •Christoph Junghans, Alexander Lukyanov, Kurt Kremer, and Denis Andrienko — Max-Planck-Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

Coarse-graining is a systematic way of reducing the number of degrees of freedom representing a system of interest. Several coarse-graining techniques have so far been developed, such as iterative Boltzmann inversion, force-matching, and inverse Monte Carlo. However, there is no unified framework that implements these methods and allows their direct comparison. We present a versatile object-oriented toolkit for coarse-graining applications (VOTCA)[1] that implements these techniques and provides a flexible modular platform for the further development of coarse-graining techniques. All methods are illustrated and compared by coarse-graining the SPC/E water model, liquid methanol, liquid propane, and a single molecule of hexane.
[1] V. Rühle, C. Junghans, A. Lukyanov, K. Kremer, D. Andrienko, Versatile Object-oriented Toolkit for Coarse-graining Applications, J. Chem. Theo. Comp. doi: 10.1021/ct900369w (2009)

CPP 11.2 Mon 16:30 Poster C

Replacement of Density Matrix Calculations by Observable Equations — •Günter Hempel — Martin-Luther-Universität, Institut für Physik, Betty-Heimann-Str, 7, 06120 Halle

The density matrix formalism is used frequently for calculations of the time evolution of spin systems, e.g. in magnetic resonance spectroscopy. The dimension of the density matrix, however, increases strongly if the number of participating spins grows. As an example, the still small system of three protons and one carbon-13 nucleus generates a 16-dimensional Hilbert space of wave functions leading to a density matrix of 256 elements. Often symmetry relations allow to conclude that some of the elements are constant or zero, others might be linearely dependent on anothers again, but nevertheless the number of differential equations we are left with might be very large. To obtain shorter systems of differential equations a method is proposed which transforms the Liouville-von Neumann-equation into a system of differential equations of observables (instead into one of matrix elements). Generally the number of differential equations of observables is essentially smaller that that of density-element equations. Examples are given which demonstrate the handling of the method and the reduction of the system of differential equations. Applications concern the spin dynamics during polarization transfer within ensembles of spin systems as well as elementary processes of spin diffusion.

CPP 11.3 Mon 16:30 Poster C

Compact magnet array for portable high-resolution NMR and Imaging — •Ernesto Danieli, Juan Perlo, Bernhard Blümich, and Federico Casanova — ITMC, RWTH Aachen University, Worringerweg 1, D-52074,Aachen, Germany

Portable NMR probes built from permanent magnets offer several advantages over conventional NMR systems. However, the inhomogeneity of the magnetic field generated by these sensors precludes their use in high resolution NMR spectroscopy and MRI. Recently we have demonstrated that the inhomogeneities of the magnetic field can be removed by providing the sensor with movable permanent magnets which allows generating and controlling harmonic field corrections by a mechanical shimming approach [1,2]. In this work we present a high-performance magnet design based on this concept, which enables us to reduce the size of the magnet keeping the field strength and the sample volume constant. In particular, it was used to build a palm size magnet working in a volume large enough to fit conventional 5 mm NMR tubes where the high field homogeneity allowed us to measure proton NMR spectra of different solvents with a resolution better than 0.16 ppm at 30 MHz. By scaling the dimensions of the magnet the same geometry was optimized to build a portable MRI scanner for imaging samples of 4 cm DSV

1. J. Perlo, F. Casanova, and B. Blümich, Science, 315 (2007) 1110-1112.

2. E. Danieli, J. Mauler, J. Perlo, B. Blumich, and F. Casanova, J. Magn. Reson., 198 (2009) 80-87

CPP 11.4 Mon 16:30 Poster C

Simultaneous investigation of morphological characteristics and crystallinity of thin nanocomposite films — •Jan Perlich[1], Jan Rubeck[1], Peter Müller-Buschbaum[2], Stephan V. Roth[1], and Rainer Gehrke[1] — [1]HASYLAB at DESY, Hamburg — [2]TU München, Physik-Department LS E13, Garching

Thin nanocomposite films formed by polymer or colloidal templates consisting of various material systems are employed in many fields such as coatings, sensors, photovoltaics, catalysis, magnetic recording and biomimetics. The preparation techniques enable the fabrication of thin films with tailor-made morphologies and specific properties. In order to correlate the characteristics of the fabricated thin films with the employed parameter settings at preparation, a detailed characterization is necessary. The simultaneous investigation of the morphological characteristics as well as the crystallinity of thin, crystalline metal oxide films is performed by small and wide angle X-ray scattering at grazing incidence (GISAXS and GIWAXS/GIXD). The small angle scattering beamline BW4 of HASYLAB, as a dedicated materials science beamline, is most suitable for such an investigation enabling the simultaneous access to an extended scattering q-range for GIWAXS. In addition, the introduction of a sample environment with defined environmental conditions, e.g. inert gas, heating and vapor treatment, enables in-situ observations of the thin nanocomposite films regarding several questions. Recent experimental data is presented and the X-ray scattering investigation is complemented in real space by surface and thin film sensitive probes.

CPP 11.5 Mon 16:30 Poster C

Status of the micro- and nanofocus x-ray scattering beamline at PETRA III — •Stephan V. Roth[1], Mottakin M. Abul Kashem[1], Gunthard Benecke[1,2], Adeline Buffet[1], Ralph Döhrmann[1], Rainer Gehrke[1], Völker Körstgens[3], Christina Krywka[4], Jannis Lehmann[5], Martin Müller[3], Peter Müller-Buschbaum[1], Kai Stassig[1], and Edgar Weckert[1] — [1]HASLYAB at DESY, Notkestr. 85, D-22607 Hamburg — [2]MPIKG, Am Mühlenberg 1, D-14476 Potsdam — [3]IEAP, CAU, Leibnizstr. 19, D-24098 Kiel — [4]GKSS, Max-Planck-Str. 1, D-21502 Geesthacht, — [5]Physik-Department E13, TU München, James-Franck-Str. 1, D-85748 Garching

The micro- and nanofocus SAXS/WAXS beamline P03 (MiNaXS), combines micro- and nano-focused x-ray beams with small- and wide-angle x-ray scattering (SAXS/WAXS). Situated at the third generation high-brilliance source PETRA III of DESY in Hamburg, Germany, MiNaXS allows for high resolution in both real and reciprocal space with beam sizes ranging from 40μm to 100nm. The low divergence offered by the high-β-undulator allows for combining ultra-SAXS geometries with such small beams. We present the current status of commissioning of the MiNaXS beamline. Strong emphasis is put on the future improvements of the various experimental in-situ scanning techniques, such as nano- and μGISAXS [1] as well as its possible combinations with high-throughput and industrial processing methods for thin film technology and fluidics [2]. [1] Roth et al., Langmuir (2009), DOI: 10.1021/la9037414 [2] Moulin et al., Rev. Sci. Instr. 79, 015109 (2008)

CPP 11.6 Mon 16:30 Poster C

PolLux - a soft x-ray nanoprobe for soft matter studies — •Andreas Späth[1], Jörg Raabe[2], Christian Hub[1], George Tzvetkov[1,2], and Rainer Fink[1] — [1]Physical Chemistry, Univ. Erlangen, Erlangen, Germany — [2]Swiss Light Source (SLS), Paul Scherrer Institut, Villigen, Switzerland

Zone-plate based x-ray microscopes offer a wide range of potential applications in fundamental and applied science, in physics, chemistry and material science or in the imaging of biosamples. The present PolLux scanning transmission x-ray microspectroscope (PolLux-STXM) is installed at a bending magnet beamline of the Swiss Light Source (SLS) operating from 260 - 1200 eV [1]. Using the latest zone-plate technology, imaging of lateral structures with 12 nm periods was achieved [2]. The available energy range is ideally suited for soft matter investigations. We will present spectromicroscopic results from various organic based materials, like organic hybrid materials (microspheres, microballoons), polymer films, organic nanocrystals or biosamples. The recent extension of the detection setup by an electron multiplier offers ad-

ditional surface-enhanced detection. Thus, we are able to combine sulk and surface sensitivity. In addition, differential phase-contrast (DPC) imaging offers another detection scheme to improve image contrast. The complementary use of the various detection schemes offers improved knowledge on the investigated soft matter samples.

The project is funded by the BMBF under contract 05 KS7WE1.

1. J. Raabe, et al., Rev. Sci. Instrum. 79, 2008, 113704.
2. K. Jefimovs, et al., Phys. Rev. Lett. 99, 2007, 264801.

CPP 11.7 Mon 16:30 Poster C

Micro total analysis system: A combination of a magnetic ratchet with giant magnetoresistance sensors — •Alexander Auge, Thomas Weiss, Dieter Akemeier, Frank Wittbracht, Alexander Weddemann, and Andreas Hütten — Uni Bielefeld, Fakultät für Physik, Universitätsstr. 25, 33615 Bielefeld, Germany

Micro Total Analysis Systems (μ TAS) on microfluidic chips is a rapidly growing field due to the large variety of possible applications like point of care diagnostics. The aim of μ TAS is to integrate all laboratory tasks on one microfluidic chip. These tasks include sample preparation, injection, manipulation, reaction, separation and detection. In this area the use of magnetic markers like beads or nanoparticles has gained importance. These markers can be selectively functionalized so that they can be attached to a variety of bioconjugates and provide reaction sites for chemical binding. One possible idea to transport, separate and detect magnetic beads is the ratchet concept. The basic idea of a ratchet is to use diffusion and a fluctuating asymmetric potential to move the magnetic markers. In this work, the ratchet is realized via a spatially periodic array of conducting lines and a magnetic out-of-plane field to create the asymmetric potential. Giant magnetoresistance sensors are placed in the potential minima of the ratchet leading to the possibility of bead detection; this allows an integrated analysis of the bead velocity. Since the bead velocity is size dependent, this enables drawing conclusions regarding e.g. bead-bacteria bindings.

CPP 11.8 Mon 16:30 Poster C

Concepts for magnetoresistive sensors and microfluidic integration — •Dieter Akemeier, Alexander Auge, Frank Wittbracht, Alexander Weddeman, and Andreas Hütten — Uni Bielefeld, Fakultät für Physik, Universitätsstr. 25, 33615

Point-of-care diagnostics is a rapidly growing field with the aim to miniaturize standard laboratory tests. Using magnetic point-of-care diagnostic devices has various advantages compared to other approaches like the direct read out of giant magneto resistance sensors, low interaction with biologic materials and low cost production.

The detection of antigens or bacteria in the continuous flow approach uses selective binding of magnetic markers on functionalized sensor surfaces located on the bottom of the flow channel. To position the particles on top of the sensor array a microfluidic structure of changing height is used. This increases the capture rate by more than 100% in comparison to a straight channel and leads to a homogeneous sensor coverage. By placing an array of 32 magnetoresistive sensors at certain position within the microfluidic system, it is possible to catch biomolecules from different starting heights on specified sensors. The experimental detection process will be discussed in detail and is compared with theoretical predictions.

CPP 11.9 Mon 16:30 Poster C

Novel techniques for the exploration of three-dimensional molecular order — •Wilhelm Kossack[1], Periklis Papadopoulos[1], Friedrich Kremer[1], Felicitas Brömmel[2], Patrick Heinze[2], and Heino Finkelmann[2] — [1]Universität Leipzig, Institut für experimentelle Physik I, Linnestr. 5, 04103 Leipzig — [2]Albert Ludwigs Universität Freiburg, Institute for Macromolecular Chemistry, Stefan Meier-Str. 31, 79104 Freiburg

Liquid Crystal Elastomers (LCE) form a novel class of materials combining the properties of liquid crystals with elastomeric networks and which can cover several application areas due to their chemical diversity. IR-Transition Moment Orientational Analysis (IR-TMOA) is employed in order to determine mean orientation and molecular order parameter of the different molecular moieties (mesogen, polymer backbone, etc.). This technique takes advantage from the specifity of the IR spectral range. Based on the measurements of the transmission dependence of polarization and an intentionally adjusted inclination of the sample numerical analysis of Maxwells-equations enables one to determine seperately the spatial orientation function of each molecular group. This provides a detailled insight into the intramolecular interactions and thus into the mechanisms governing order.

CPP 11.10 Mon 16:30 Poster C

Time resolved 3D orientation spectroscopy of functionalized perylene bisimide (PBI) molecules — •Richard Börner[1], Danny Kowerko[2], Stefan Krause[2], Christian von Borczyskowski[2], and Christian G. Hübner[1] — [1]Institute of Physics, University of Lübeck, Ratzeburger Allee 160, 23538 Lübeck, Germany — [2]Center for Nanostructured Materials and Analysis, Chemnitz University of Technology, 09107 Chemnitz, Germany

Fluorescence detection on a single molecule level has been used to investigate interconversions between different molecular conformational states of perylene bisimide (PBI) type molecules, which are subject to intramolucular dynamics due to flexible bay groups [2]. This intramolecular dynamics may lead to spectral diffusion, fluorescence intensity and/or lifetime fluctuations and changes in the orientation of the emission dipole. Therefore, a simultaneous measurement of all parameters is mandatory. To this end, we show a detection scheme that allows for simultaneous determination of the full three-dimensional emission dipole orientation, fluorescence intensity, the fluorescence lifetime and the emission spectra of single fluorescent molecules. The obtained ms time resolution for the orientation determination [1] in comparison to other methods enables a simultaneous access on fast intramolecular conformational dynamics accompanied by changes in the orientation of the fluorescence emission dipole that is in the long axis of the dye PBI molecule.

[1] J. Hohlbein & C. G. Hübner, JCP, 129, 094703 (2008)
[2] D. Kowerko et al., Molecular Physics, 107 (2009)

CPP 11.11 Mon 16:30 Poster C

Local thermomechanical characterization of phase transitions on polymers using heated SFM-probes — •Thomas Fischinger, Martin Laher, and Sabine Hild — Department of Polymer Science, Johannes Kepler University Linz, Altenbergerstrasse 69, 4040 Linz, Austria

Thermal analysis methods are important instruments for polymeric research, however, up to now mainly bulk properties are detected. Local thermal analysis (LTA) based on scanning probe microscopy (SPM) allows the probing of melting and glass transition temperatures on a 100 nm length scale. To understand local mechanisms for temperature-induced phase transitions in polymers quantitative measurements of characteristic thermomechanical properties such as glass transition and melting temperatures as well as temperature dependent elastic and loss modulus and thermal expansion coefficients in nanoscale volumes are required. Since conventional LTA is insensitive to changes in the dissipative properties in the materials a new approach based on the combination of acoustic atomic force microscopy band excitation detection and a heated tip probe is for the unambiguous detection of changes in resonance frequency and tip-surface dissipation. In the first step, an appropriate temperature calibration method has been established using carboxylic acids with defined melting points to correlate the deflection signal or amplitude and frequency changes with the temperature of the probe. Bases on this, the glass transition temperature will be determined on microscopic scale. The opportunities given by this method are demonstrated in selected model polymeric systems.