CPP 15: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods II

Time: Monday 17:15–19:00 Location: ZEU/0255

CPP 15.1 Mon 17:15 ZEU/0255

Deep Learning-Driven Grazing Incidence Small-Angle X-ray Scattering Data Processing for Nanostructure Characterization — •Yufeng Zhai[1], Jungui Zhou[1], Shachar Dan[1], Julian Heger[2], Benedikt Sochor[1,3], Arno Jeromin[4], Wenbo Wang[5], Wolfgang Parak[5], Sarathlal Koyiloth Vayalil[1,6], Thomas Keller[4,5], Andreas Sitierle[4,5], Alexander Hexemer[3], Peter Müller-Buschbaum[2], and Stephan V. Roth[1,7] — [1]DESY, Hamburg, Germany — [2]TUM, Garching, Germany — [3]ALS/LBNL, California, United States — [4]CXNS, Hamburg, Germany — [5]UHH, Hamburg, Germany — [6]UPES, Dehradun, India — [7]KTH Stockholm, Sweden

Nanostructured thin films formed via nanoparticle deposition or self-assembly exhibit diverse morphologies that are crucial for their functional properties. Grazing-incidence small-angle X-ray scattering (GISAXS) provides detailed structural information on such systems, but conventional model-based fitting remains limited by simplified assumptions and convergence difficulties. We employ the distorted wave Born approximation (DWBA) to simulate a wide range of two-dimensional GISAXS patterns, which are used to train convolutional neural networks (CNNs) for predicting nanoparticle size distributions. The trained models demonstrate robust performance on both simulated and experimental data, providing a faster and more flexible alternative to traditional fitting. In addition, we have developed a graphical user interface (GUI) that integrates conventional fitting routines with our deep learning framework, providing a user-friendly platform for rapid GISAXS analysis.

CPP 15.2 Mon 17:30 ZEU/0255

Chirp-DMA for expanded frequency and reduced aging — •Juan Pablo Segovia Gutiérrez[1], José Alberto Rodríguez Agudo[2], Jan Haeberle[2], Dominic Oppen[2], Jörg Läuger[2], and Natalie Germann[1] — [1]University of Stuttgart, Stuttgart, Germany — [2]Anton Paar Germany GmbH, Ostfildern, Germany

Optimal Fourier Rheometry (OFR), or Chirp rheometry, is an advanced technique that uses a continuous, sine wave-shaped stress/strain signal characterized by an exponential frequency increase. This approach is important for measuring rapidly time-evolving soft materials, where conventional frequency sweeps are impractical; their slow, sequential data acquisition often fails to capture fast structural changes before the material itself mutates. A key advantage of Chirp is its ability to drastically reduce measurement time, making it highly effective at low and very low frequencies. This speed is essential to circumvent undesirable material aging, for instance in the dehydration observed in hydrogels, which modifies properties during long acquisition times. Conventionally, Chirp has been implemented using standard plate-plate geometries. The novelty of this study is the implementation of Chirp within a Dynamic Mechanical Analysis (DMA) setup utilizing extension and torsion modes. This permits the characterization of soft, fragile materials outside the typical rheometer configuration. By combining this novel Chirp-DMA approach with conventional sweeps on gellan gum/alginate hydrogels, we extend the practical frequency range and prove that Chirp recovers true viscoelastic moduli, thereby eliminating dehydration-induced effects.

CPP 15.3 Mon 17:45 ZEU/0255

PIERS-Based Mechanistic Insights into PVC Micro- and Nanoplastics Degradation on Ag Nanoflake-TiO2 Platform — •Olugbenga Ayeni[1], Josiah Ngenev Shondo[2], Tim Tjardts[3], Sinan Şen[4], Franz Faupel[3], Salih Veziroglu[3], Oral Cenk Aktas[3,4], and Tayebeh Ameri[1] — [1]Chair for Composite Materials, Department of Materials Science, Kiel University, Germany. — [2]Department of Energy Conversion and Storage, Technical University of Denmark, Denmark. — [3]Chair for Multicomponent Materials, Department of Materials Science, Kiel University, Germany. — [4]Department of Orthodontics, University Hospital of Schleswig-Holstein (UKSH), Kiel, Germany.

Conventional characterization techniques such as FTIR and SERS have been applied to Polyvinyl chloride (PVC) micro- and nanoplastics (MNPs) degradation, but they lack the combined real-time sensitivity and photocatalytic functionality needed to probe early-stage PVC-MNPs degradation. In this work, we report the use of Photo-induced enhanced Raman spectroscopy (PIERS) technique under continuous UV illumination to monitor the degradation of PVC-MNPs in real time on a highly active photocatalytic platform based on Ag nanoflakes (Ag NFs) grown on TiO2 thin films. Our PIERS-based approach reveals the chemical transformations and structural disorder occurring in the PVC-MNPs backbone within 10 min of UV irradiation. Our results establish PIERS as a promising mechanistic probe for tracking real-time PVC degradation pathways at the nanoscale. This study advances the mechanistic understanding of plastic degradation at the nanoscale.

CPP 15.4 Mon 18:00 ZEU/0255

Exploring Colloidal Kinetics Using DLS — •Mohit Agarwal and Jiaxing Sun — Swabian Instruments GmbH, Stuttgart, Germany

The kinetic behavior of colloidal and soft matter systems arises from particle diffusion, aggregation, and structural rearrangement, which collectively determine how microstructures evolve over time. Accurate characterization of these dynamics is crucial for understanding nonequilibrium phenomena such as gelation, crystallization, and phase separation in complex fluids. Conventional experimental techniques often lack the temporal and angular resolution needed to resolve these fast and heterogeneous processes in their native state, especially when multiple relaxation mechanisms coexist. We present a time-resolved, multi-angle Dynamic Light Scattering (DLS) technique that records individual photon arrival events in real-time across multiple scattering angles. This configuration enables angle-dependent temporal correlation analysis with improved sensitivity to both short-time diffusive motions and long-time relaxation processes that reflect evolving particle interactions. By employing complete photon statistics rather than time-averaged intensity correlations, the method captures transient fluctuations and kinetic transitions in colloidal suspensions. Measurements on well-defined colloidal dispersions reveal subtle temporal variations in particle dynamics and aggregation behavior that remain inaccessible with conventional single- or multi-angle goniometer-based DLS. The technique establishes a robust framework for real-time, multi-scale investigation of kinetic processes in colloidal and soft matter systems.

CPP 15.5 Mon 18:15 ZEU/0255

The Power of One Oxygen: How a Single Atom Alters the Field Evaporation of Liquid Crystals — •Kuan Meng, Sebastian Eich, and Guido Schmitz — University of Stuttgart, Institute for Materials Science, Heisenbergstr. 3, 70569 Stuttgart, Germany

In this study, we established a cryo-atom probe tomography (cryo-APT) workflow to investigate how the presence of a single oxygen atom alters the field evaporation behavior of two structurally similar liquid crystals: 8CB and 8OCB. Both compounds exhibited over 70% intact molecular retention and comparable fragmentation patterns.

Mass spectra revealed that the oxygen in 8OCB hinders the formation of extended cyanobiphenyl fragments across the linkage and promotes full cleavage of the alkyl chain. In contrast, 8CB allows the formation of longer backbone fragments. Spatially, 8CB evaporated mainly as intact molecules across both crystalline and smectic domains. 8OCB, however, evaporated predominantly as small fragments in low volume-density domains while as larger fragments or intact molecules in the high volume-density regions, which are suspected to crystalline and smectic phases, respectively. Further structural validation is required.

This work illustrates how cryo-APT enables the characterization of the molecular structure of organic liquid systems and demonstrates that even a single oxygen atom can fundamentally alter their field evaporation pathways. It further proposes a tunable fragmentation strategy to investigate molecular orientation in soft matter at an unprecedented resolution.

CPP 15.6 Mon 18:30 ZEU/0255

Depth-resolved cathodoluminescence for mapping exciton diffusion in rubrene thin film polymorphs — •Heiner Thiersch[1,2], Jonas Schröder[1], Anna-Lena Hofmann[1], Wooik Jang[1], Nora Engelmann[1], Fritz Henke[1], Maximilian F. X. Dorfner[3], Shu-Jen Wang[4], Frank Ortmann[3], Johannes Benduhn[1,2], Ellen Hieckmann[1], and Karl Leo[1] — [1]IAPP, TU Dresden, Germany — [2]DZA Görlitz, Germany — [3]Dep. of. Chem., TU München, Germany — [4]Dep. of. Phys., HKBU, China

The exciton diffusion length (L_D) is a key parameter in opto-electronic devices, as it governs the transport and recombination of photogenerated excitons. However, accurately measuring L_D remains challenging due to the limited penetration depth and lateral resolution of conventional techniques such as photoluminescence quenching and transient absorption spectroscopy. Here, we will introduce a novel approach for L_D determination based on quenching processes observed by depth-resolved cathodoluminescence (CL) measurements with highly localized excitation. The method combines CL experiments with kinetic Monte Carlo simulations and a diffusion model derived from Fick's second law. Applied to the organic semiconductor rubrene-renowned for its high hole mobility in single crystals- the technique yields L_D values ranging from 50 to 100 nm across different thin-film polymorphs. The results provide new insights into the exciton dynamics of rubrene and present a new methodological tool for accurate L_D characterization in semiconductors.

CPP 15.7 Mon 18:45 ZEU/0255

Towards Theoretical UV/Vis Spectra with Experimental Accuracy - Functional Errors and Thermal Broadening — •Robert Strothmann[1], Johannes T. Margraf[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]University of Bayreuth, Bayreuth, Germany

First principles methods like time-dependent density-functional theory (TD-DFT) can be used to predict molecular UV/Vis spectra relying on a number of approximations such as the choice of functionals, the description of solvation, as well as the treatment of thermal broadening. For the latter, simple (smeared) line spectra or structural ensembles obtained within the harmonic approximation are the most common choices. With the rise of machine learning interatomic potentials (MLIP) prohibitively costly *ab initio* molecular dynamics (MD) simulations can be replaced with similarly accurate MLIP MDs. This allows a detailed comparison of these approaches for a large number of systems for the first time.

In this talk, we benchmark predicted UV/Vis spectra against experimental references. To this end, the agreement with a curated set of literature reported spectra for diverse organic molecules in various solvents is assessed in terms of full spectral overlap, beyond a "peak to peak" comparison. We emphasize the influence of functional choice and thermal sampling approaches (e.g. harmonic vs. anharmonic), as well as the role of different conformers. How important each of these effects is and how it affects computational cost will be studied with the goal of providing best practise guidelines.