CPP 12: French-German Session: 2D Materials, Thin Films and Interfaces I

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

Invited Talk CPP 12.1 Mon 15:00 ZEU/0255

Multifunctional films by tailoring chemistry and morphology of polymer brushes at the nanoscale — •Petra Uhlmann and Alexander S. Münch — Leibniz-Institut für Polymerforschung Dresden, Hohe Strasse 6, 01069 Dresden

Functional polymer thin films, like stimuli-responsive polymer brushes or cross-linked polymer networks, are a group of smart surface coatings which are beneficial for the design of intelligent interfaces. One emphasis of our work is the synthesis of polymer brushes as a toolbox for the creation of specific surface functions and stimuli-responsive layers using a bottom-up approach. For many technical applications control and switching of wettability is a key property. In this contribution it will be shown how tailored co-polymers containing zwitterionic phosphorylcholine groups (MPC) and benzophenone (BPO) as anchoring and UV cross-linking units can be used to create multifunctional films with easy-to-clean, anti-fog, anti-fouling and anti-icing properties. For the achievement of the desired surface functions the control of not only the wettability, but also other thin film properties like thickness and degree of swelling, are crucial and require the respective optimization of the chemical polymer composition and the degree of crosslinking. For verification and adjustment of the interfacial and thin film properties atomic force microscopy (AFM), infrared spectroscopy (ATR-FTIR), contact angle measurements, and in-situ spectroscopic ellipsometry were used and correlated with respective coatings performance and sustainability tests.

CPP 12.2 Mon 15:30 ZEU/0255

Increase in elastic modulus of thin elastic films and membranes containing rigid inclusions - revisiting Einstein's relation in two dimensions — •Konstantin Zisiadis and Andreas Menzel — Otto-von-Guericke-Universität Magdeburg

Elastic matrices with well-separated inclusions can be described by effective elastic moduli obtained via homogenization methods. Probably the most basic relation for dilute systems is the Einstein equation $\eta_{\text{eff}} = \eta(1 + 2.5\phi)$. We consider the two-dimensional geometry of an elastic matrix in two dimensions with two-dimensional elastic moduli as counterparts to the three-dimensional case. Both plane-stress and plane-strain geometries are treated. We employ a generalized stresslet formalism. Our derived formulae for the effective moduli of the two-dimensional geometry are expressed using the two-dimensional elastic moduli for an arbitrarily compressible matrix. We find that the plane-stress and plane-strain equations for the effective moduli have the same form, while the associated two-dimensional moduli differ. Our results are consistent with previous research based on different approaches. For an incompressible matrix, we recover the known effective shear modulus $\mu_{\text{eff}} = \mu(1 + 2\phi)$.

We acknowledge support by the German Research Foundation (DFG) through Research Unit FOR 5599 on structured magnetic elastomers.

CPP 12.3 Mon 15:45 ZEU/0255

Structure and optical properties of donor-HATCN blends — •Gianfranco Melis, Dmitry Lapkin, Ainur Abukaev, Alexander Hinderhofer, and Frank Schreiber — Universität Tübingen, Tübingen, Germany

Organic thin films made of molecular semiconductors have the potential to advance the range of functional materials for technological progress. In this regard, electron donor-acceptor complexes (DAC) show unique physical properties at specific ratios due to their non-linear structure-property-composition dependence. A systematic study across the full mixing range is therefore essential to understand how structure and optical response evolve with composition.

Compositional-gradient thin films were prepared in a custom-built organic molecular beam deposition chamber by co-depositing donor materials—diindenoperylene (DIP), pentacene (PEN), coronene (COR), picene (PIC), α-sexithiophene (α-6T), zinc phthalocyanine (ZnPc), and perylenetetracarboxylic acid bis(propylimide) (PTCDI-C_3)—with the prospective non-fullerene acceptor hexaazatriphenylenehexacarbonitrile (HATCN). Grazing-incidence wide-angle X-ray scattering (GIWAXS), atomic force microscope (AFM), and UV-Vis absorption spectroscopy were applied to study and correlate structural and optical properties with the donor-acceptor stoichiometry. New absorption bands appear below the optical bands of pure materials at specific stoichiometric compositions, together with different surface morphologies and the formation of new mixed structural phases.

CPP 12.4 Mon 16:00 ZEU/0255

Optimized Phenyl-Modified g-C3N4/ZnO Hybrid Thin Films: Structural and Optical Insights — •Sahar Aghapour Ghourichay[1,2], Morgan Le Du[2], David P. Kosbahn[2], Guangjiu Pan[2], Hagen Uebele[2], Thomas Baier[2], Jinsheng Zhang[2], Lyuyang Cheng[2], Pier Carlo Ricci[1], and Peter Müller-Buschbaum[2] — [1]Department of Physics, University of Cagliari, Cittadella Universitaria, Monserrato, Italy — [2]TUM School of Natural Sciences, Chair for Functional Materials, Garching, Germany

Phenyl-modified graphitic carbon nitride (PhCN)/ZnO hybrid thin films were fabricated with different PhCN loadings to investigate the influence of interface engineering on their structural and optical properties. UV-vis reflectance results show that the film containing 1 mL PhCN exhibits the lowest reflectance and the strongest absorption in the visible region. Photoluminescence analysis confirms that this optimized film has significantly reduced emission intensity, indicating more effective charge separation. XRD, AFM, and GIWAXS measurements reveal improved crystallinity and enhanced nanoscale ordering of ZnO in the presence of moderate PhCN content. SEM/EDS mapping verifies uniform hybrid formation, and XPS provides evidence of interfacial chemical interaction. Overall, controlled PhCN incorporation effectively tunes the optical response and nanoscale structure of PhCN/ZnO thin films, offering useful insights for photocatalytic and optoelectronic applications.

CPP 12.5 Mon 16:15 ZEU/0255

Machine Learning for Grazing-Incidence Diffraction (GID): from Raw Data to Crystalline Structure — •Dmitry Lapkin, Ainur Abukaev, Ekaterina Kneschaurek, Mikhail Romodin, Constantin Völter, Vladimir Starostin, Alexander Hinderhofer, and Frank Schreiber — Universität Tübingen

The optimization of novel materials in the form of thin films for specific applications requires the appropriate structural characterization methods. X-ray and neutron scattering techniques, such as grazing incidence small- and wide-angle X-ray/neutron scattering (GISAXS/GIWAXS/GISANS) or grazing-incidence diffraction (GID), offer the ultimate spatial resolution and high surface sensitivity, making them indispensable tools for thin film studies. At the same time, advancements in X-ray and neutron sources, in conjunction with developments in area detector technologies, enable the recording of several terabytes of raw two-dimensional detector data within a single experiment. Conventional methods of analyzing the GID data are severely under-paced compared to the data generation rates, representing a significant bottleneck and leaving much of the measured data unanalyzed. To make the thin film studies more efficient and increase the amount of analysed and published GID data that can be reused, we are developing a comprehensive machine learning based data analysis pipeline that goes from raw detector patterns to the corresponding crystalline structures. This pipeline comprises several stages, including data preprocessing and reduction, Bragg peak identification and refinement, and crystal structure determination.

Invited Talk CPP 12.6 Mon 16:30 ZEU/0255

Thin-film and interface properties in energy conversion devices unveiled by X-rays — •Marcus Bär — Department Interface Design, Helmholtz-Zentrum Berlin für Materialien und Energie GmbH (HZB), Berlin, Germany — Energy Materials In-Situ Laboratory Berlin, HZB, Berlin, Germany — Department of Chemistry and Pharmacy, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — Department of X-ray Spectroscopy at Interfaces of Thin Films, Helmholtz-Institute Erlangen-Nürnberg for Renewable Energy, Berlin, Germany

This invited talk will present recent advances in the characterization of the chemical and electronic structure of interfaces and thin films that are central to modern energy-conversion technologies. A combination of X-ray spectroscopies enables non-destructive, depth-resolved insight into composition, chemical structure as well as bonding and energy-level landscapes across complex and often (deeply) buried interfaces.

Interfacial intermixing, interlayer formation, oxidation processes, and energy-level alignment govern charge transport and recombination in energy conversion materials and devices. Illustrative case studies will be used to demonstrate how changes (e.g., in the thin-film deposition process) affect interfacial chemistry and electronic structure, highlighting the importance of the ability to probe interface properties as a prerequisite for deliberate interface design. In addition, the talk will outline recent progress in establishing dedicated sample environments allowing for in-situ and operando studies opening new pathways for understanding dynamic interface phenomena.