CPP 29: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods III

Time: Tuesday 14:00–15:30 Location: ZEU/0255

CPP 29.1 Tue 14:00 ZEU/0255

Towards Evolved Sensing Applications for Organic Photonic Devices Utilizing Room-Temperature Phosphorescence — •Sebastian Kaiser, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics (IAP), Technische Universität Dresden

Photonic devices function through the absorption and emission of light, making them independent of electricity or other influences. This trait is vital for sustainable advances in imaging, sensing, information storage, and anticounterfeiting. Programmable luminescent tags (PLTs) exemplify this by utilizing the oxygen-sensitivity of organic room-temperature phosphorescence (RTP) for controllable switching of the device's light output under UV illumination. [1, 2]
Optimizing the homogeneity and reproducibility of photonic thin-film devices, paired with use-case-tailored layer compositions, allowed us to develop a new, advanced UV light-sensing application. The thin-film nature of PLTs, especially their flexibility and transparency, combined with a freely scalable sensor area, enables a broader range of use cases than common detectors can achieve. The combination of these unique device characteristics opens the way for new sensing applications for purely photonic devices.

[1] Gmelch et al., Science Advances 2019. aau7310
[2] Tsiko et al., Communications Chemistry 2025, 025-01620-0

CPP 29.2 Tue 14:15 ZEU/0255

Synergistic and unique information reveals multicentre bonding and geometry — •Kyunghoon Han, Miguel Galleogos Gonzalez, and Alexandre Tkatchenko — University of Luxembourg, Luxembourg, Luxembourg

Classical bonding measures and entropy maps are mostly pairwise, obscuring cooperative effects. We introduce a Partial Information Decomposition of bond character built from standard density-functional and coupled-cluster data. Fragment electron- and spin-number distributions along a coordinate define a simple label (covalent, ionic, multicenter), and information about that label is separated into redundant (shared), unique (single-fragment), and synergistic (joint-only) parts. Treating bond character as a geometric response, small perturbations yield a synergy profile that pinpoints where cooperation emerges and how it evolves. The profile rises at the onset of sharing in diatomic hydrogen, is maximal for the central bond of bicyclo[1.1.1]propellane only when the bridgeheads and the three methylene groups are taken together, and peaks at the square geometry of cyclobutadiene before dropping with bond alternation. Benchmarks against density, orbital, energy, and machine-learning descriptors show where PID adds explanatory power and, for ordinary two-center bonds far from dissociation, why it is near-zero with detectable exceptions only when the two atoms are the same.

CPP 29.3 Tue 14:30 ZEU/0255

Utilizing Immediate Phosphorescence in Organic Photonic Devices for Rewritable Information Storage and Oxygen Sensing — •Lucy Winkler, Sebastian Schellhammer, and Sebastian Reineke — Dresden Integrated Center for Applied Physics and Photonic Materials (IAPP) and Institute of Applied Physics (IAP), Technische Universität Dresden

Programmable luminescent tags (PLTs) are photonic devices that offer simple and versatile solutions for reversible information storage and food labeling by using the oxygen-sensitive phosphorescent emission from organic emitters embedded in polymer matrices [1]. Conventional PLTs fabricated by spin-coating under ambient conditions exhibit oxygen-quenched phosphorescence in their initial state, requiring photoactivation to consume oxygen in the active layer and switch on emission. However, these PLTs show inconsistent activation between the initial and subsequent writing processes, significantly limiting their controlled reusability for practical applications [2]. To better understand activation cycles and identify potential improvements, different fabrication workflows in oxygen-free environments were tested. While activation behavior remains similar to conventional devices, these fabrication approaches enable creation of activated PLTs with an initial switched-on state that could serve as simple oxygen detectors, for example, in vacuum packaging integrity monitoring.
[1] Thomas, H. et al. Adv. Mater. 36, 2310674 (2024).
[2] Tsiko, U., et al. Commun Chem 8, 274 (2025).

CPP 29.4 Tue 14:45 ZEU/0255

Solution to the current paradox of anomalous underscreening in electrolytes — •Esther Ohnesorge, Thomas Tilger, Michalis Tsintsaris, Hayden Robertson, and Regine von Klitzing — Department of Physics, Technische Universität Darmstadt, Darmstadt, 64289, Germany

Since colloidal dispersions have a significant importance in our daily life, it is of special interest to get a deeper understanding of which interfacial forces govern their stability and how this stability can be tailored.

For aqueous electrolyte solutions, DLVO theory is a powerful and well-established framework to describe these interactions at low and intermediate ionic strengths. In contrast, the situation at high ionic strength is less understood and the main methods for direct force measurements give inconsistent results. Whilst the surface force apparatus (SFA) provides clear evidence for a re-entrance of repulsion in the highly concentrated regime (termed underscreening) for a wide range of different electrolytes [1], similar observations were not possible with the atomic force microscope (AFM) to date [2]. In this presentation we will examine the reason of these fundamental differences. Specifically, in an attempt to explore experimental screening lengths across a wide suite of electrolyte concentrations, we demonstrate the experimental parameters dominating the occurrence of anomalous underscreening and a comprehensive understanding of this long-debated phenomenon. [1] DOI: 10.1103/PhysRevLett.119.026002 [2] DOI: 10.1016/j.jcis.2022.05.004

CPP 29.5 Tue 15:00 ZEU/0255

Thermal properties of a knotted diblock copolymer ring — •Neda Abbasi Taklimi[1], Franco Ferrari[1], Marcin Radoslaw Piatek[1], and Luca Tubiana[2] — [1]Institute of Physics, University of Szczecin, Wielkopolska15, 70-451 Szczecin, Poland — [2]INFN-TIFPA, Trento Institute for Fundamental Physics and Applications, Via Sommarive 14, I-38123 Trento, Italy

The phase transitions and geometrical properties of diblock copolymers have been studied extensively; however, few studies have addressed knotted structures under varying monomer distributions and solvent quality. Here, we present a computational study of how topological constraints and block lengths affect the behavior of a single diblock copolymer ring. We used the Wang-Landau Monte Carlo algorithm and a coarse-grained model on a simple cubic lattice with an implicit solvent to explore thermal and structural properties. In the AB model, A-type monomers are self-repulsive, B-type monomers are self-attractive, and AB interactions are neutral; the solvent is good for A-type and poor for B-type monomers at low temperatures.

We computed key properties, including heat capacity, radius of gyration of individual blocks and the whole ring, number of contacts (AA, BB, AB), and knot length. Our results reveal several phase transitions for specific monomer distributions and topologies. Subtle changes in monomer distribution lead to transitions between knotlocalization and delocalization at low temperatures, driven by the competition between entropic and energetic contributions to the free energy.

CPP 29.6 Tue 15:15 ZEU/0255

A Systematic Multiscale Study of Bio-Based Polymers for Novel Food Packaging Systems — •Andoni Ugartemendia, Alessandro Mossa, and Giorgia Brancolini — Institute of Nanoscience, CNR-NANO S3, via G. Campi 213/A, 41125 Modena, Italy

Recently, monolayer materials of bio-based polymers have gained increased attention to develop more sustainable packaging systems.[1] In this regard, rational in silico design has become essential to predict novel polymers and reduce experimental workload. However, the computational modeling of these materials poses a great challenge since their dynamics span over different time scales.[2] To bypass this issue, in this work we propose a modular multiscale computational protocol to study linear polymers from ab initio to coarse grained (CG) dynamics. In the first part, we derive a full atomistic force field (FA-FF) from DFT data and carry out FA-MD simulations for its validation. In the second step, all structural properties are passed to a database to parametrize a CG-FF with the iterative Boltzmann inversion (IBI).[3] Lastly, large scale CG-MD simulations are run for a final validation of the CG-FF. This methodology is applied first to PET, a polymer widely used in the packaging industry, as well as to emerging bio-based polymers such as PEF and PLLA.

[1] V. Guillard, et al., Front. Nutr., 2018, 5, 121. [2] R. B. Bird, R. C. Armstrong, O. Hassager, Dynamics of Polymeric Liquids. Volume 1: Fluid Mechanics, 2nd ed. (Wiley-Interscience, United States, 1987). [3] A.P. Lyubartsev, et al., J. Chem. Theory Comput. 2013, 9, 1512.