CPP 26: French-German Session: 2D Materials, Thin Films and Interfaces II

Time: Tuesday 14:00–15:30 Location: HÜL/S386

Invited Talk CPP 26.1 Tue 14:00 HÜL/S386

Investigating lignin graphitisation depending on botanical source and extraction method — Lucie Dieval[1], Phuthiphong Ouitrakoon[2], Robert Hunter[2], Sébastien Schaefer[3], Louis Hennet[3], Erik Elkaim[4], Julie Ruellou[5], Milo S. P. Shaffer[2], Agnieszka Brandt-Talbot[2], and •Pascale Launois[1] — [1]LPS, CNRS/Université Paris Saclay, France — [2]Imperial College, UK — [3]ICMN, CNRS/University of Orléans, France — [4]Synchrotron SOLEIL, France — [5]ESRF, France

Lignins, plant-derived macromolecules, are promising carbon sources from a sustainable development perspective. Here, we study the transformations of various lignins into turbostratic carbon or graphite, consisting of stacked graphene sheets.

The lignin powders were heated at temperatures between 1000 and 2730°C. Analyses were performed ex-situ using X-ray scattering (XRS) and Raman spectroscopy, which confirmed XRS results. XRS data were analysed combining analyses in reciprocal space and in direct space with Pair Distribution Function. The dimensions of the carbonaceous crystalline domains formed from lignins are determined as a function of temperature, as well as the stacking mode of their graphene sheets. We find that all studied lignins transform into turbostratic carbon, with no evidence for intermediate stackings towards graphite. Different sizes of crystalline domains are evidenced depending on the lignin form. One lignin presents relatively large sizes both for the graphene layers and in the stacking direction at a temperature as low as 1300°C, a most promising finding for future applications.

CPP 26.2 Tue 14:30 HÜL/S386

Atomistic Origin of Photoluminescence Quenching in Colloidal MoS_2 and WS_2 Nanoplatelets — •Surender Kumar[1], Markus Fröhlich[2], Stefan Velja[1], Marco Kögel[2], Onno Strolka[2,3], André Niebur[3], Samuell Ginzburg[4], Muhammad Sufyan Ramzan[1], Jannik C. Meyer[2], Jannika Lauth[2,3], and Caterina Cocchi[1] — [1]Friedrich-Schiller-Universität Jena, Germany — [2]Eberhard Karls University of Tübingen, Germany — [3]Leibniz University of Hannover, Germany — [4]University of Cambridge, UK

Large chemical tunability and strong light-matter interactions make colloidal transition metal dichalcogenide nanostructures particularly suitable for light-emitting applications. However, ultrafast exciton decay and quenched photoluminescence limit their potential. Combining femtosecond transient absorption spectroscopy with first-principles calculations on MoS_2 and WS_2 nanoplatelets, we reveal that the observed sub-picosecond exciton decay originates from edge-located optically bright hole traps [1]. These intrinsic trap states stem from the metal *d*-orbitals and persist even when the sulfur-terminated edges are hydrogen-passivated. Notably, WS_2 nanoplatelets show more localized and optically active edge states than their MoS_2 counterparts, and zigzag edges exhibit a higher trap density than armchair edges. The nanoplatelet size dictates the competition between ultrafast edge-trapping and slower core-exciton recombination, and the states responsible for exciton quenching enhance catalytic activity.

[1] S. Kumar, et al., arXiv:2511.19077 (2025)

CPP 26.3 Tue 14:45 HÜL/S386

Data-driven exploration of thermal and elastic properties in covalent organic framekworks — •Aleksander Szewczyk[1], Leonardo Medrano Sandonas[1], David Bodesheim[1], Bohayra Mortazavi[2], and Gianaurelio Cuniberti[1] — [1]TUD Dresden University of Technology, 01062 Dresden, Germany — [2]Leibniz Universität Hannover, Welfengarten 1A, 30167 Hannover

Covalent organic frameworks (COFs) are a class of advanced materials that can be precisely engineered for diverse applications, including catalysis, flexible electronics, and sensors. However, COFs synthesised experimentally often exhibit a variety of structural defects and grain boundaries, which affect their properties. Because of their large and complex structure, COFs pose a considerable challenge for traditional *ab-initio* methods. Machine learning interatomic potentials (MLIPs) can be used to significantly accelerate property calculations, while retaining near *ab-initio* accuracy. Our team have parametrised an MLIP using the MACE architecture and a dataset of non-equilibrium confirmations of 2D COFs. We assessed the transferability of the MACE model computing atomic forces and phonon dispersions of unseen COFs, and compared these results to ReaxFF and reference data by Density Functional Theory using VASP code. Using the parametrised model, we explore the effect of defects and grain boundaries on thermal and elastic properties of COFs.

CPP 26.4 Tue 15:00 HÜL/S386

PNIPAM Microgel-Stabilized Foam Films: Effect of Crosslinking Content — •Luca Mirau, Joanne Zimmer, Kevin Gräff, Matthias Kühnhammer, and Regine von Klitzing — Institute for Condensed Matter Physics, TU Darmstadt, Germany

Aqueous foams find widespread application in fields such as cosmetics, the food industry, oil recovery and fire-fighting. Their stabilization requires the presence of surface-active molecules or colloidal particles. In this study, thermoresponsive microgels (MGs) composed of poly(N-isopropylacrylamide) (PNIPAM) with varying crosslinker contents are applied as foam stabilizers, resulting in temperature-sensitive foams. Foam films serve as the fundamental building blocks of foams. The structuring of MGs within these films is analyzed using the Thin Film Pressure Balance (TFPB) technique. Foam films are formed within a pressure chamber, and their thickness is determined through interferometric methods under a light microscope. The foam films display an inhomogeneous structure, characterized by network-like, several 100nm thick regions containing MGs, interspersed with thin MG-depleted zones less than 100nm thick. We show how the cross-linker density of the microgels affect the MG layering within these thick network regions, influencing the film thickness. Another question we answer is how the MG-free areas are stabilized.

CPP 26.5 Tue 15:15 HÜL/S386

Irreversible protein adsorption on mobile surfaces: control and modelling of surface density and in-plane mobility through molecular crowding — Wanchung Chiang[1], Lionel Bureau[1], Ralf Richter[2], Galina Dubacheva[1], and •Delphine Debarre[1] — [1]Grenoble-Alpes University, France — [2]University of Leeds, UK

Adsorption of proteins onto surfaces has been the focus of a wealth of experimental, theoretical and numerical studies but surprisingly little is known on the dynamics of protein adsorption on fluid surfaces.

In this study, we consider irreversible adsorption of streptavidin, a protein with a very strong affinity for its ligand biotin, onto a lipid bilayer incorporating biotin-terminated lipids, a widely-used model to build biomimetic surfaces. We show that after the initial, rapid adsorption phase, a slower, logarithmic continuous adsorption can lead to surface densities much larger than in the absence of surface diffusion. Simultaneously, we quantify the lateral diffusion of the adsorbed proteins, which drops sharply and can be tuned continuously over two orders of magnitude depending on surface density.

We then adapt free-volume theories to two dimensions to rationalize our findings and bridge the gap between in-plane diffusion and adsorption dynamics. Beyond a better understanding of adsorption onto mobile surfaces, our data paves the way towards biomimetic surfaces incorporating mobility control of functional groups.