CPP 14: Emerging Topics in Chemical and Polymer Physics, New Instruments and Methods

Time: Tuesday 9:30–11:15 Location: H39

CPP 14.1 Tue 9:30 H39

Where is the Water? — •Maximilian Fuchs[1,2], Eduardo Machado Charry[1,2], Gregor Böhm[1,2], Roland Resel[1], and Karin Zojer[1,2] — [1]Institute of Solid State Physics, NAWI Graz, Graz University of Technology, Austria — [2]Christian Doppler Laboratory for Mass Transport through Paper, Graz University of Technology, Austria

The take up of liquid water by paper is a complex interplay between capillary transport and swelling of cellulose-lignin-based fibers. Though paper is a convenience product used every day, little is known how swelling affects the pore space between fibers and the subsequent transport within it. We used X-ray microcomputed tomography to monitor the spread of water in-situ. The sequence of 3D-images, segmented by a neural network, traces the time-dependent progression of swelling and liquid transport up to one hour after the application of water. We find that water not only swells the fiber walls, but also expands the pore space between the fibers. Even more remarkable is that there is no liquid water in the pores between the fibers of the examined paper. Rather, liquid water was found exclusively in the fiber lumen.

CPP 14.2 Tue 9:45 H39

Rational Design of Novel Photoswitches with Generative Models — •Robert Strothmann, Christian Kunkel, Johannes T. Margraf, and Karsten Reuter — Fritz-Haber-Institut der MPG, Berlin, Germany

The sheer vastness of chemical spaces poses a daunting challenge to molecular discovery through high-throughput screening based on exhaustive sampling. Generative models (GMs) are an emerging machine learning (ML) approach that enables a more guided discovery. Implicitly learning chemical design rules from large reference data sets and suitable descriptors of a targeted functionality, GMs directly propose promising, yet diverse candidates.
Here we explore the use of GMs for the design of novel molecular photoswitches. In order to guarantee the desired functionality in the generated molecules, we specifically employ scaffold decoration methods that append chemically meaningful side-groups to a predefined photochromic core. In a second step, the creation process needs to be conditioned towards performant switching capabilities. In the absence of sufficient corresponding experimental reference data, this conditioning is based on synthetic first-principles data. To this end, we discuss computationally efficient descriptors assessing addressability and robustness.

CPP 14.3 Tue 10:00 H39

Transferable hidden variables in sequence space learned by transencoder neural networks — •Marco Werner — Institut Theorie der Polymere, Leibniz-Institut für Polymerforschung Dresden, Germany

The relation between chemical sequences and the properties of polymers is investigated using artificial neural networks with a bottleneck layer of neurons. By training such AutoEncoder networks to translate between sequence and property (TransEncoder[1]), one may identify variables that control the physical relationship behind. Here, networks were trained to predict the effective free energy landscape of a copolymer interacting with a lipid membrane depending on its sequence of hydrophilic and hydrophobic monomers. TransEncoders that were split into separate encoder-decoder channels have learned to decompose the free energy into independent components that were physically meaningful. For instance, they reflect theoretical concepts such as solutions of the Edwards equation. Sequence-complete data sets for training were obtained via Rosenbluth sampling of single chains in a given density field. It is demonstrated that once the sequence patterns were learned based on the large data set for chain length $N = 14$, a small number of ~ 20 examples was sufficient to transfer-learn the prediction to a more detailed simulation model with explicit lipids and solvent (accuracy $0.5k_BT$). The results open a perspective to physics-informed inverse searches, for instance, for copolymer sequences leading to the smallest translocation time through a membrane. [1] M. Werner, ACS Macro Lett. 10, 1333 (2021).

CPP 14.4 Tue 10:15 H39

Improved virtual orbitals for the calculation of X-ray absorption spectra for organic molecules — •Rolf Würdemann[1] and Michael Walter[2,3] — [1]Freiburger Materialforschungszentrum, Freiburg, Germany — [2]Freiburger Zentrum für interaktive Werkstoffe und bioinspirierte Technologien, Freiburg, Germany — [3]Fraunhofer-Institut für Werkstoffmechanik, Freiburg, Germany

X-ray absorption spectroscopy (XAS) is an element specific local probe used for the analysis of materials. One way to compare and interpret experimentally measured spectra is to perform ab initio calculations of XAS spectra for molecules in given geometries. This opens a way to distinguish between different isomers and gain a deeper understanding of the bonding situation.

Common ways to calculate XAS spectra by density functional theory (DFT) either utilize fractional charges in the frozen cores or restrict the state-space of linear time-dependent DFT. In our contribution we examine the possibility to utilize the combination of range-separated functionals (RSF) with Huzingas improved virtual orbitals to calculate XAS spectra. This combination has been successful in the calculation of charge transfer excitations[1].

[1] R. Würdemann, M. Walter, J. Chem. Theory Comput. 2018, 14, 7, 366

CPP 14.5 Tue 10:30 H39

Transport of organic volatiles through paper: physics-informed neural networks for solving inverse and forward problems — •Alexandra Serebrennikova[1,4], Raimund Teubler[2,4], Lisa Hoffellner[2,4], Erich Leitner[2,4], Ulrich Hirn[3,4], and Karin Zojer[1,4] — [1]Institute of Solid State Physics, TU Graz, Petersgasse 16, Graz, 8010, Austria — [2]Institute of Analytical Chemistry and Food Chemistry, TU Graz, Stremayrgasse 9/II, Graz, 8010, Austria — [3]Institute of Bioproducts and Paper Technology, TU Graz, Inffeldgasse 23, Graz, 8010, Austria — [4]Christian Doppler Laboratory for mass transport through paper, Petersgasse 16, Graz, 8010, Austria

Transport of volatile organic compounds (VOCs) through porous media with active surfaces takes place in many applications, e.g., in cellulose-based materials for packaging. To date, mathematical models proposed in literature for this complex process are scarce and have not been systematically compiled together with experimental data.

Based on a model for water-vapor transport through paper (Ramarao et al. (2003)), we propose to describe transport of VOCs via diffusion in pores and sorption to fibers. It is key to determine the necessary material parameters for the model. Using experiments for that is challenging, as the related system of non-linear PDEs does not offer analytical solutions.

We demonstrate for dimethyl sulfoxide and n-tetradecane, how combining experimental concentration data with physics-informed neural networks yields these parameters as solution of an inverse problem.

CPP 14.6 Tue 10:45 H39

STED-Inspired Sub Diffractional Cationic Lithography — •Sourav Islam[1], Marco Sangermano[2], and Thomas Klar[1] — [1]Institute of Applied Physics, Johannes Kepler University Linz, 4040 Linz, Austria — [2]Department of Applied Science and Technology, Politecnico Di Torino, Torino, Italy

Cationic polymerization has come out as a low cost, efficient, biocompatible alternative to radical polymerization because of lower toxicity of the monomers, lower shrinkage stress, no oxygen inhibition. Although the mechanism of cationic polymerization is well understood(1), the knowledge about two-photon induced cationic polymerization is still insufficient. In our work, we try to fill the void in the knowledge of two photon induced cationic polymerization and the scope of STED-inspired (2) sub diffractional lithography. 3,4-Epoxycyclohexylmethyl 3,4 epoxycyclohexanecarboxylate (CE) was used as monomer and Triarylsulfonium hexafluoroantimonate salts and 2-Isopropylthioxanthone (ITX) were used as onium salt and photosensitizer, respectively. 110fs laser pulses of 780nm wavelength were used to write two-photon polymer lines with a feature size of 315nm. Furthermore, 60% suppression of polymerization was achieved using an additional 660nm continuous beam overlapped with 780nm beam. To obtain further reduction of the feature size, a donut shaped beam profile was produced by installing a 2-pi phase plate in the 660 nm

beam path. This way, lines of 195 nm feature size were achieved. 1.M. Sangermano Pure and Applied Chemistry, 84, 2089 (2012). 2.Fischer, Wegener, Opt. Mat. Exp. 1, 614 (2022)

CPP 14.7 Tue 11:00 H39

Photoluminescence spectroscopy for the detection of microplastics - the Nile Red approach — •Srumika Konde, Stefan Brackmann, Marina Gerhard, and Martin Koch — Department of Physics and Material Sciences Center, Philipps-University of Marburg, Germany

For the detection and classification of microplastics, most researchers commonly use FTIR or Raman spectroscopy. These state-of-the-art methods are, however, laborious, cost-intensive, and time-consuming. To establish a less arduous and inexpensive approach, we propose photoluminescence-based multispectral imaging. Based on the parallel research in our workgroup, we have found that the autofluorescence of plastics lies predominantly in the UV region. To accommodate the identification in the visible region we use a solvatochromic dye called Nile Red. PLE/PL spectra of stained plastics and stained natural materials have been analyzed to determine the right excitation and emission windows for building an imaging system. This analysis has been performed using LDA (linear discriminant analysis). Based on our analysis we propose a system consisting of a blue excitation LED, an RGB camera, and two bandpass filters which would yield about 98% accuracy in isolating plastics from natural materials.