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Controlling the order in colloidal crystals by progressively changing the shape of particles

M. Lattuada^{1,2}, J. Smart^{1*}

¹Department of Chemistry, University of Fribourg, Chemin du Musée 9, 1700 Fribourg (CH), ²
Marco.lattuada@unifr.ch

Monodisperse colloidal particles are known to self-organize into an ordered crystalline phase with a face-centered cubic structure when subject to strong repulsive interactions at sufficiently high concentrations, showing structural colors when particles with a size comparable to the wavelength of visible light are used. This structural color shows an angular dependence in highly ordered photonic crystals, which decreases when a low degree of disorder is present in the crystal structure. Once the disorder in the crystal becomes too large, the structural color is lost.

To control the extent of disorder in colloidal crystals, we decided to investigate the formation of colloidal crystals using slightly non-spherical particles. This has been achieved by preparing highly monodisperse dimpled particles synthesized from standard polystyrene colloids with controlled dimple size and depth. In this manner, various colloidal crystals made of particles with small and large dimples have been prepared, as shown in the figures below.

The structure of these crystals was meticulously investigated using focused ion-beam scanning electron microscopy (FIB-SEM) to recover the position of all particles. This thorough examination revealed that an increase in the dimple size leads to a progressive loss of ordered structure and structural coloration. Brownian Dynamics simulations were then performed to gain a deeper understanding of the mechanism leading to the formation of disorder, confirming the progressive loss of order as the particle shape deviates from sphericity. These findings underscore the profound impact of particle shape on the crystallization of colloids, a significant contribution to our understanding of this field.

Multifunctional Photonic Microparticles via Block Copolymer Self-Assembly: From Structural Color to Magnetically Responsive Optical Materials

A. Dodero^{1,2}, G. Mazzotta^{3,2*}, N. R. Schwarz^{1,2*}, S. Bertucci^{1*}, R. Schobinger^{1*}, D. Peddis^{4*}, D. Comoretto^{4*}, U. Steiner^{1,2*}

¹Adolphe Merkle Institute, University of Fribourg, Chemin des Verdiers 4, 1700 Fribourg, Switzerland, ²NCCR Bio-Inspired Materials, Chemin des Verdiers 4, 1700 Fribourg, Switzerland, ³Department of Chemistry, University of Fribourg, Chemin du Musée 9, 1700 Fribourg, Switzerland, ⁴Department of Chemistry and Industrial Chemistry, University of Genoa, Via Dodecaneso 31, 16146 Genoa, Italy

Controlling structural color through scalable, precise, and multifunctional material design remains a key objective in the development of next-generation photonic systems. Here, we present a robust fabrication platform based on the confined self-assembly of block copolymers (BCPs) within emulsion droplets, enabling the production of photonic microparticles with lamellar architectures and vivid structural color. The process allows precise tuning of the photonic bandgap across the visible spectrum by modulating domain periodicity and refractive index contrast through supramolecular additives and low molecular weight swelling agents.¹

This approach addresses key challenges in photonic material design by combining structural robustness, spectral tunability, and compatibility with scalable emulsification methods. It further enables the incorporation of functional nanomaterials – such as quantum dots, plasmonic, and magnetic nanocrystals – into specific block copolymer domains, resulting in hybrid microparticles that integrate photonic coloration with tailored emission,² plasmonic,³ or magnetic properties. Additionally, we demonstrate the fabrication of anisotropic, rod-like photonic microparticles by tuning emulsion conditions and embedding magnetic nanoparticles into the BCP matrix. These rods exhibit orientation-dependent color and can be dynamically aligned using external magnetic fields, enabling programmable optical responses.

The resulting materials offer a promising platform for a wide range of applications. In particular, we demonstrate the formulation of water-based structural color coatings by combining photonic microparticles with broadband absorbers and polymeric binders, yielding vibrant, fade-resistant paints suitable for industrial application on surfaces, packaging, textiles, and cosmetics. Beyond coatings, these materials show strong potential in sensing, optical tagging, anti-counterfeiting, display technologies, and wearable devices where their tunable, angle-independent, or magnetically reconfigurable coloration can be exploited for dynamic, responsive, and secure photonic systems.

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A Highly Conductive Halospinel Cathode for All-Solid-State Batteries

J. F. Baumgärtner^{1,2}, D. Isler^{1,2*}, D. Chernyshov^{3*}, K. V. Kravchyk^{1,2*}, M. V. Kovalenko^{1,2*}

¹ETH Zürich, ²Empa Dübendorf, ³ESRF Grenoble

To meet the growing demands of modern energy storage, cathode active materials (CAMs) in Li-ion batteries (LIBs) not only need to offer high energy density, but also enable fast charge and discharge.^[1] To this end, CAMs must facilitate both rapid electronic and ionic transport at the lattice scale, since chemical diffusion will be rate-limited by the slower species (Figure a, b). While oxospinel meets these criteria and are therefore widely employed in state-of-the-art LIBs, we demonstrate that halospinels offer greatly enhanced transport properties and enable the incorporation of earth-abundant transition metals such as iron (Figure c, d).^[2] Using $\text{Li}_{2-x}\text{FeCl}_4$ ($0 < x \leq 1$, LFC) as a model system, we show that its intrinsically high ionic-electronic conductivity allows for all-solid-state batteries (ASSBs) with micron-sized CAM particles, achieving exceptional areal capacity ($> 2 \text{ mA h cm}^{-2}$) at practical current densities (0.5 mA cm^{-2}) and extended cycle life of 200 cycles (Figure e). Our findings position LFC as a commercially viable CAM, paving the way for cost-effective, high-performance ASSBs.

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Organic halide perovskite solar devices incorporating electroactive interlayers: computational insights and design principles from DFT

A. Vezzosi¹, V. Slama^{1*}, V. Carnevali^{1*}, G. AlSabe^{2*}, M. Grätzel^{2*}, U. Röthlisberger^{1*}

¹Laboratory of Computational Chemistry and Biochemistry, EPFL, Switzerland, ²Laboratory of Photonics and Interfaces, EPFL, Switzerland

The advancement of metal halide perovskite solar cells (PSCs) hinges on achieving high performance while ensuring long-term operational stability. In this study, we present a comprehensive investigation—both experimental and theoretical—of two complementary approaches to interfacial engineering in perovskite solar devices, centered on the design and implementation of electroactive organic spacer molecules.

We explore the possibility to introduce electroactive organic spacers at the perovskite/ETL interface inverted (p-i-n) PSC architectures to mitigate non-radiative recombination while simultaneously enhancing charge extraction.[1] Density functional theory (DFT) and ab-initio molecular dynamics (AIMD) simulations support experimental observations by revealing how these spacers facilitate interfacial charge transfer and stabilize the interface. We further investigate their role in fullerene-free architectures, identifying electronic design criteria for spacer molecules that enable both passivation and efficient transport.

Also, we examine the incorporation of π -conjugated aryl-acetylene-based spacers into hybrid layered (2D/3D) perovskite structures.[2] Spacers such as (4-ethynylphenyl)methylammonium (BMAA) and buta-1,3-diyne-1,4-diylbis(4,1-phenylene)dimethylammonium (BDAA) not only passivate surfaces and inhibit the transition to non-photoactive phases, but also participate actively in charge transport. Experimental characterization shows that mixed-dimensional perovskite devices incorporating these spacers achieve power conversion efficiencies up to 23% and exhibit superior operational stability. Theoretical analyses highlight favorable energy level alignment and strong orbital delocalization through the π -conjugated backbones for BDAA, enabling effective coupling with charge transport layers.

Together, these findings provide design principles for multifunctional electroactive interlayers that simultaneously enhance stability, suppress recombination, and facilitate efficient charge transport.

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Polymer Analysis from Cradle to Grave and BeyondO. Skarsetz¹¹TA instruments / Waters GmbH, Helfmann-Park 10, 65760 Eschborn Germany

Polymers are ubiquitous in materials science, yet their full potential can only be realized through comprehensive analytical approaches spanning their entire lifecycle. This talk presents an integrated methodology for polymer analysis from synthesis to material performance. We begin with thermal characterization techniques such as Thermogravimetric Analysis (TGA) and Differential Scanning Calorimetry (DSC), which provide critical insights into polymer structure, thermal stability, and phase transitions. These methods enable the correlation of molecular structure to material properties. The focus then shifts to mechanical evaluation of macroscopic polymer materials using tensile and fatigue testing, essential for assessing strength, elasticity, as well as long-term durability in real applications under cyclic load. By combining thermal and mechanical analyses, we demonstrate how a holistic understanding of polymer properties can inform material design. This talk aims to inspire cross-disciplinary collaboration and highlight the analytical possibilities available to researchers in polymer science.

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MatChem PhD Student Award Ceremony 2025**B. Brand**¹, M. Yarema^{2*}¹ZHAW Wädenswil, ²ETH Zurich

The Division of Materials Chemistry of the SCS is proud to honor the winners of the 2025 MatChem PhD Student Awards. The program is sponsored by Sika and Vigor and the awardees receive a prize money of CHF 1'000 each. The award ceremony takes place during the [MatChem morning parallel session](#) at the [SCS Fall Meeting](#) in Zurich on September 4, 2025. After the ceremony both winners will present their projects in a 5min flash presentation.

The board of the MatChem Division as well as the SCS Head Office like to congratulate the two winners:

Dr. Till Schertenleib (group of Wendy Lee Queen, EPFL Lausanne) currently working as Postdoc at the University of Copenhagen

PhD thesis: „A local structure perspective on metal-organic frameworks“.

Dr. Yuan-Zi Xu (group of Victor Mougel, ETH Zurich) currently working as Postdoc at the ICFO, Barcelona Institute of Science and Technology

PhD thesis on nitrogen oxides (NO_x and nitrate) with a focus on exploring new electrocatalysts for nitrate reduction.

MatChem PhD Student Award

The prizes are given for outstanding PhD thesis' that were performed in the area of materials chemistry within Switzerland between January 2024 and May 2025.

<https://scg.ch/matchem>

Highly Uniform Colloids of Metallic and Intermetallic Nanocrystals

M. Yarema¹

¹ETH Zurich, Dept. Information Technology and Electrical Engineering, Gloriastrasse 35, 8092 Zürich, Switzerland - yaremam@ethz.ch

It is difficult to overestimate the importance of metals and alloys, and nanoscale dimensionality adds even more functions and unicity to these materials. Captured by unfolding and rich application space, our research group studies metallic and intermetallic nanocrystals in the form highly uniform colloids. Specifically, we have developed several monoatomic nanocrystals (e.g., Bismuth, Indium, and Gallium) with unprecedented quality for size control and monodispersity^{[1],[2],[3]} and studied their colloidal synthesis by in-situ synchrotron-based methods.^[4] Our synthetic efforts have provided a pathfinder for a range of applications, including 3D self-assemblies, stamped electrodes, or Li-ion battery anodes.^{[1],[2],[5]} Recently, we have extended beyond monoatomic metals and developed the first universal approach for high-quality intermetallic nanocrystals (**Figure 1**).^[6] Our method employs an amalgamation reaction at the surface of nanocrystals and unlocks up to a 1000 of new intermetallic nanocrystals with unprecedented quality for size uniformity, composition control, and phase purity. Starting from monometallic seeds (e.g., Ni, Cu, Pd, Ag, or Au), we carry out a thermal decomposition of metal-amides (e.g., Ga, In, or Zn amides) to dispatch low-melting metals to the surface of nanocrystals. This is followed up by the amalgamation process, i.e., an efficient way of alloy formation, in which a liquid metal diffuses into solid metal forming a bimetallic composition or intermetallic compound. One of the highlights is the remarkable kinetics of metal alloying during amalgamation, taking advantage of the high diffusivity of liquid metal component. Therefore, the amalgamation reaction is fast, convenient, and it takes only a couple of minutes to form homogeneous bimetallic nanocrystal. Consequently, the amalgamation synthesis is faster than detrimental mass transfer processes, such as Ostwald ripening. Thus, particle sizes and size uniformity of intermetallic nanocrystals are directly inherited from the high-quality monometallic seeds. Furthermore, the nanoscale amalgamation reaction shows excellent universality for Zn, In and Ga bimetallic nanocrystals and our method allows reaching various phases within the same bimetallic composition. Taking the example of Au-Ga, we were able to synthesize a wide range of compositions.^[5] We prepare nanocrystals of Ga-doped *fcc*-Au, hexagonal Au₇Ga₂, low-symmetry AuGa, and cubic AuGa₂ phases simply by tuning the amount of added liquid Ga (i.e., the amount of Ga amide salt). Interestingly, we also observe two-phase samples, indicating miscibility gaps in bimetallic phase diagrams and providing means to reconstruct thermodynamic phase equilibria at the nanoscale.^[7]

Figure 1: Schematics of nanoscale amalgamation reaction for high-quality intermetallic nanocrystals.

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Excited-state charge transfer interaction in a benzothiadiazole/benzodithiophene supramolecular assembly

I. Kolly¹, P. Debnath^{2*}, S. M. Langenegger^{1*}, A. Cannizzo^{2*}, R. Häner^{1*}, S. X. Liu^{1*}

¹Department of Chemistry, Biochemistry and Pharmaceutical Sciences, W. Inäbnit Laboratory for Molecular Quantum Materials and WSS-Research Center for Molecular Quantum Systems, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland, ²Institute for Applied Physics, University of Bern, Sidlerstrasse 5, CH-3012 Bern

Benzodithiophene/benzothiadiazole-based trimers have been synthesized and characterized. In aqueous conditions, the oligomers self-assemble into distinct nanostructures, which was observed by AFM and DLS measurements. UV-vis spectroscopy was performed and showed, that the supramolecular polymers (SPs) are formed at 20°C, whereas at 80 °C the oligomers are disassembled. Fluorescence spectroscopy revealed that the emission of the electron-accepting benzothiadiazole moiety is efficiently quenched through the presence of the electron-donating benzodithiophene moiety. This excited-state charge transfer interaction seems to take place via photoinduced electron transfer, which was further analyzed by TAS measurements and confirmed the interaction of the non-conjugated donor-acceptor moieties upon photoexcitation.^[1] The charge transfer interaction in SPs can be altered by changing the donor-acceptor sequence in the trimer. A-D-A and D-A-D trimers are compared to get a closer insight into this phenomenon.

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A Practical and Robust Approach to Determining the Experimental Minimal Formula of Metal-Organic Frameworks

J. Pulparayil Mathew¹, C. Simms^{2,3*}, D. Salazar Marcano^{1*}, E. Dhaene^{1*}, T. Parac-Vogt^{2*}, J. De Roo^{1*}

¹Department of Chemistry, University of Basel, Mattenstrasse 22, 4058 Basel, Switzerland, ²Department of Chemistry, KU Leuven, Celestijnenlaan 200F, 3001 Leuven, Belgium, ³Department of Chemistry, University of Antwerp, Universiteitsplein 1, 2610 Wilrijk, Belgium

Metal-organic frameworks (MOFs) have been one of the most advancing classes of materials in the past few years, with immense potential in the field of catalysis,¹ gas storage,² drug delivery,³ water purification,⁴ etc. However, the fundamental aspect of determining the precise chemical composition of the synthesised MOFs is lacking sufficient attention, although it is crucial for many advanced applications, such as catalysis.

In this work, we present a simple yet robust methodology to derive the minimal formula of the synthesised MOF material.⁵ To achieve this, we combine Nuclear Magnetic Resonance (NMR) spectroscopy, Thermogravimetric analysis (TGA), and UV-Vis spectroscopy. We investigated the previously used methodologies that solely rely on TGA and demonstrated why the assumptions that were made in this technique are not justified. We further dive deep into the use of NMR to quantify the different organic molecules present in the framework. We have also shown the crucial influence of digestion methods and relaxation time on the accurate determination of the minimal formula. We also highlight the often-overlooked presence of residual inorganic species, particularly chloride and nitrate ions originating from the precursors such as ZrCl₄ or ZrOCl₂ (for Zr-based MOFs), or cerium ammonium nitrate (for Ce-based MOFs). These residues can remain embedded within the framework in significant quantities, impacting properties such as catalytic activity and framework stability. Our methodology provides a quantitative means of identifying and accounting for these species.

To align MOF characterisation with practical applications, we introduce the concept of “experimental molar mass”, reflecting the true chemical identity of the MOF as synthesised and handled under laboratory conditions. We used our methodology to derive the experimental minimal formula of MOF-808(Zr), UiO-66(Zr), UiO-66(Ce), MOF-5(Zn), MIL-125(Ti), and MIL-100(Fe), to show the generality of our technique. We further extended our work to amorphous coordination networks, such as an Al-BDC MOF with no information on its crystal structure. Our work focuses on obtaining a fully charge-balanced and chemically feasible minimal formula. This work thus lays the foundation for a more rigorous, transparent, and application-relevant reporting of MOF compositions and serves as a critical step towards the rational design and development of MOFs in both fundamental research and industrial contexts.

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Exploring the Synthesis and Applications of Two-dimensional Polymers

V. Lupu^{1,2}, D. Opriş^{1,2*}

¹Laboratory for Functional Polymers, EMPA Dübendorf, Überlandstrasse 129, 8600, Dübendorf, Switzerland, ²Department of Materials, ETH Zurich, Vladimir-Prelog-Weg 5, Zurich 8093, Switzerland

For most of the history of chemistry, polymeric materials were strictly known as 1D, monomers strung together in a linear fashion to form long chains. Recently, new methods and monomers were developed that allow the growth of two-dimensional graphene-like polymeric structures, known as 2D polymers (2DPs). Due to their 2D nature, these polymers are naturally highly ordered, gaining novel applications as nanoporous membranes for use in separating specific molecules (CO₂ capturing, for example), in batteries (as anionic conductors), as extremely high surface area catalyst supports, ultrathin coatings and many more. However, the current array of 2D monomers is very narrow, as few molecules fit the packing and symmetry criteria required for these materials. One such class are 3-fold star-shaped styryl-pyrylium salts. These monomers present excellent crystal packing for topochemical polymerization via π - π stacking. At the same time, the pyrylium ring facilitates exfoliation via charge repulsion and provides an easy post-polymerization modification route via its high reactivity towards nucleophiles. Previously, such a monomer was obtained with bulky t-butyl groups close to the reactive site of the pyrylium ring^[1], severely limiting the options for modification due to steric bulk. We report a new monomer with isopropyl groups that can be used to obtain, for example, N-alkyl-pyridinium containing 2DPs, which have proven to be excellent anionic conductors in batteries, having been reported to enable capacity retention of 93% after 1000 cycles^[2]. This monomer proves vastly pluripotent in its functionalization, amine groups can be inserted for CO₂ capture or even bulky substituents for adjustable pore size. The compound has proven easy and relatively inexpensive to make on a large scale, while its crystals can be grown to relatively large sizes from common solvents.

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Low-Temperature Depolymerization of Polymethacrylamides

V. Lohmann¹, G. R. Jones^{1*}, A. A. Kroeger^{2*}, N. P. Truong^{1*}, M. L. Coote^{2*}, A. Anastasaki^{1*}

¹Laboratory of Sustainable Polymers, Department of Materials, ETH Zürich, ²Institute for Nanoscale Science and Technology, College of Science and Engineering, Flinders University

The depolymerization of polymers synthesized by reversible deactivation radical polymerization (RDRP) has recently garnered significant attention due to its potential for recovering monomer at low temperatures. However, current reports focus solely on polymethacrylates, significantly limiting applications, scope, and fundamental understanding. Although polymethacrylamides are highly valued for their excellent biocompatibility, anti-bacterial properties, and water solubility, their chemical recycling remains experimentally unattainable, irrespective of their synthesis method (i.e. free radical, RDRP, anionic, etc.). Herein, we present the first example of thermal reversible addition-fragmentation chain-transfer (RAFT) depolymerization of various polymethacrylamides, regenerating monomers at high yields. Central to our work was the identification of two key weaknesses associated with polymethacrylamides, namely (i) insufficient end-group activation, and (ii) premature end-group loss at higher temperatures, leading to compromised monomer yields and low depolymerization rates. These challenges were bypassed via the addition of commercially available radical initiators, resulting in faster reactions and higher percentages of recovered monomer at as low as 90 °C. The broad applicability of this method was further demonstrated by its compatibility with various RAFT-agents, and the possibility to depolymerize a crosslinked hydrogel. Our work expands the depolymerization scope of high-value materials beyond polymethacrylates and shines a light on intriguing thermodynamic and kinetic insights.

V. Lohmann, G.R. Jones, A.A. Kroeger, N.P. Truong, M.L. Coole, A. Anastasaki, *Angewandte Chemie International Edition*, 2025, e202425575.

Synthesis of large transition metal dichalcogenide single crystals with flat surfaces by selected vapor growth

J. N. Tangermann¹, F. O. von Rohr^{1*}

¹Department of Quantum Matter Physics, University of Geneva

Transition metal dichalcogenides (TMDs) provide a versatile platform for exploring quantum phenomena, enabled by their layered van der Waals structures and the coexistence of competing electronic states such as superconductivity and charge density waves. However, synthesizing high-quality crystals remains challenging: chemical vapor transport (CVT) often produces inconsistent morphologies, while chemical vapor deposition (CVD) can introduce substrate-induced strain.

In this work, we present selected vapor growth (SVG) as a scalable alternative for producing large, exfoliable single crystals of TaS₂, TaSe₂ and NbSe₂. By applying a controlled temperature gradient in a muffle furnace and utilizing iodine-assisted transport, we obtained crystals exceeding 1 cm in size with flat, well-defined surfaces. SVG enables precise control over growth conditions and crystal morphology, making it a promising route for fabricating high-quality TMDs for both fundamental research and device integration.

Synthesis and characterization of polysiloxanes with photoswitchable dielectric properties

M. S. Beccard^{1,2}, T. R. Venkatesan^{3*}, M. Bauer^{3*}, D. M. Opris^{3*}

¹Functional Polymers, Empa, Swiss Federal Laboratories for Materials Science and Technology (EMPA), 8600 Dübendorf, Switzerland, ²Eidgenössische Technische Hochschule Zürich (ETHZ), 8092 Zurich, Switzerland, ³Empa

This study presents a novel photoswitchable polysiloxane elastomer's synthesis, characterization, and potential applications. The photoswitching functionality is introduced by grafting via esterification arylazopyrazole (**AAP**) on the polysiloxane chains, followed by cross-linking. The **AAP** undergoes a reversible *trans-cis* isomerization upon exposure to UV light, returning to the *trans* form under green light or thermal conditions. A lithium salt was incorporated to enhance the ion conductivity of the samples, which was processed into thin films on interdigitated electrodes.

In the *trans* form, the photoactive **AAP** binds to the lithium ions. Conversely, in the *cis* form, the ions are liberated, thereby enabling the polymer to alter its properties in response to light. Using an interdigitated electrode setup, we measured dielectric permittivity, loss tangent ($\tan(\delta)$), and conductivity while exposing the sample to light. These properties exhibit an increase upon light exposure and revert when the light is turned off. The observed changes are attributed to two simultaneous phenomena: heating of the samples when exposed to light of any wavelength and *trans-cis* isomerization together with a cleavage of the complex of the **AAP** molecules under UV light. It has been demonstrated that the ionic conductivity can be reversibly switched over 100 cycles.

This capability suggests potential applications in electronic devices that could reversibly modify their ionic conductivity when exposed to UV light.

Disentangling Size and Yield of Cesium Lead Bromide Perovskite Nanocrystals with Cesium Precursor Engineering

Y. Berezovska^{1,2}, V. Sekula^{1*}, N. Romanyuk^{1*}, D. Dirin^{1,2*}, M. Kovalenko^{1,2*}

¹ETH Zürich, Switzerland, ²Empa - Swiss Federal Laboratories for Materials Science and Technology, Switzerland

Lead halide perovskite (LHP) nanocrystals (NCs) recently gained significant attention as classical and quantum light sources. Their photoluminescence is highly dependent on NC size, making its precise control essential for optimizing NC performance. The room temperature synthesis introduced by Akkerman et al.¹ demonstrated that reduced activity of the PbBr_2 enables improved control over nucleation and growth of NCs and allows the synthesis of monodisperse NCs with sizes ranging from 3 to 13 nm. However, the synthesis of small NCs in this case is achieved by strong dilution of the precursors. As a result, 3-4 nm small NCs can be synthesized only at low yields (10-50 mg at 1 L reaction scale).

To increase the yield of small CsPbBr_3 NCs, we venture into tuning the activity of the second precursor – cesium diisooctylphosphinate – by replacing it with cesium salts of custom-synthesized dialkyl phosphinic acids, monoalkyl phosphinic acids, and phosphonates.² We show that cesium precursor reactivity can be used to tailor nucleation and growth rates with shorter linear chains and branched tails consistently resulting in smaller NCs than their longer and linear counterparts. Cesium precursor presents a new way to control the CsPbBr_3 NC growth mechanism and allows us to decouple the size and yield of the synthesized NCs.

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Exploration of Monocompound Hybrid Metal Halides as Scintillators for Fast Neutron Radiography

A. Bhardwaj^{1,2}, K. Sakhatskyi^{1,3*}, A. Sakhatska^{1,3*}, P. Trtik^{4*}, Y. Padniuk^{1,3*}, Y. Wu^{5*}, Y. Kominko^{1,3*}, K. Han^{6*}, Z. Xia^{6*}, Z. Xia^{6*}, M. Strobl^{4*}, A. L. Rogach^{5*}, S. Yakunin^{1,3*}, M. Kovalenko^{1,3*}

¹Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, Switzerland,

²DECTRIS Ltd., Taefernweg 1, 5405 Baden-Daettwil, Switzerland, ³Laboratory of Thin Films and

Photovoltaics Empa-Swiss Federal Laboratory for Material Science and Technology, Dübendorf, Switzerland, ⁴

Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institute, 5232 Villigen PSI, Switzerland, ⁵

Department of Materials Science and Engineering and Centre for Functional Photonics, City University of Hong Kong, 83 Tat Chee Avenue, Hong Kong S.A.R. 999077, China, ⁶State Key Laboratory of Luminescent Materials

and Devices, Guangdong Provincial Key Laboratory of Fiber Laser Materials and Applied Techniques, School of Physics and Optoelectronics, South China University of Technology, Guangzhou 510641, China

Fast neutron radiography remains an indispensable method for imaging objects such as fossils and nuclear fuel assemblies constituting a dense mix of light and heavy elements. The current detection technology which rely on two-phased scintillator composed of ZnS microparticles embedded in polypropylene(PP) matrix, suffers from its inability to achieve high light yield (LY) without degradation in spatial resolution. This limitation stems from the inefficient energy conversion due to independent neutron absorption in PP and reduced excitation probability in low volumetric fraction of ZnS luminophores in PP:ZnS. In this work, we overcame this challenge by utilizing a monocompound zero-dimensional hybrid metal halide $\text{TPP}_2\text{MnBr}_4$ scintillator which due to its homogenous structure exhibit a four-fold higher LY compared to PP:ZnS demonstrating a superior recoil proton energy utilization. Furthermore, radiography measurements from $\text{TPP}_2\text{MnBr}_4$ scintillator results in spatial resolution of one line per millimeter, comparable to that of PP:ZnS.

Bridgman Growth of Li_3InCl_6 Single Crystals Enables Investigation of the Crystal Structure – Ionic Conductivity Relationship

C. Černe^{1,2}, A. Kanak^{1*}, J. F. Baumgärtner^{1,2*}, K. V. Kravchyk^{1,2*}, M. V. Kovalenko^{1,2*}

¹Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, CH-8093 Zürich, Switzerland, ²Laboratory for Thin Films and Photovoltaics, Empa – Swiss Federal Laboratories for Materials Science & Technology, CH-8600 Dübendorf, Switzerland

Li_3InCl_6 (LIC) is a promising solid-state electrolyte (SSE) to enable high-energy-density lithium batteries due to its high oxidative stability, compatibility with high-voltage cathode active materials,¹ and high ionic conductivity of up to 2 mS cm^{-1} .² LIC (C2/m) has a layered structure with alternating Li^+ and In^{3+} layers within a distorted *fcc* Cl^- sublattice. Due to the paramount importance of the precise Li^+ and In^{3+} sub structure, as well as stacking faults, for the bulk ionic conductivity, and the potential to modify the cation-sub structure by changing the synthetic method, a detailed analysis of differences in Li^+ and In^{3+} ordering as a function of synthetic method needs to be carried out. While cation ordering and stacking faults can theoretically be deconvoluted in diffraction experiments, they require highly crystalline LIC samples which have not been obtained so far.³

In this context, we recently developed a procedure to grow LIC single crystals (SCs) with the Bridgman method, providing a reference with minimized cation disorder and stacking faults. LIC SCs were grown in a vertical two-zone Bridgman furnace with a temperature gradient up to $20\text{--}30 \text{ K cm}^{-1}$. Peritectic-like crystallization behavior was observed during the crystal growth: LiCl phase crystallizes first, followed by formation of the target LIC phase and residual InCl_3 . Powder XRD revealed LiCl impurity in the lower region of the LIC phase. Adjustment of the growth speed to $0.5\text{--}0.3 \text{ mm h}^{-1}$ and cooling rate to $7\text{--}3 \text{ K h}^{-1}$ allowed to obtain SCs of high quality, confirmed by optical inspection under the polarization microscope. Laue diffraction showed that the crystal growth direction is perpendicular to the *bc* plane.

In our future work we aim to explore the *synthesis method – crystal structure – ionic conductivity* relationship for the LIC SSE. Precise Li^+ and In^{3+} sub structure of the SC sample and samples prepared by high-energy ball milling route with and without a subsequent annealing step and by solid-state high temperature synthesis, will be determined using single-crystal and powder neutron diffraction experiments.

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PEF/PET-starch hydrogels from recycled sources for shrimp farm's wastewater treatment

S. T. Cerqua¹, E. Bonora^{1*}, P. Kongseng^{2*}, S. Chantarak^{2*}, C. Brändli^{1*}

¹Institute of Materials and Process Engineering, Zurich University of Applied Sciences, Technikumstrasse 9, Winterthur, CH, ²Division of Physical Science, Prince of Songkla University, 15 Karnjanavanich Rd, Hat Yai, TH

Polyethylene terephthalate (PET) is one of the most widely used polymers, found in numerous commercial applications.[1] Nowadays, companies are shifting to recycled PET (rPET), cutting greenhouse gas emissions by 45–55% and saving 440–520 PJ of energy annually.[2] A promising bio-based alternative is polyethylene 2,5-furanoate (PEF), made from 100% plant-based building blocks: plantMEG™ and FDCA.[3] PEF offers improved shelf life, light-weighting, and better thermal resistance, making it a strong sustainable candidate to replace PET. Effective waste management is key for PEF's global adoption. One approach is converting PEF waste into hydrogels for wastewater treatment.[4] This project aims to develop novel PEF- and furan-based hydrogels and convert PET waste into biodegradable hydrogels by forming crosslinked networks with natural-based polymers. The developed hydrogels will be used for the treatment of wastewater (dyes, heavy metals, antibiotics, etc.) from shrimp farming and aquaculture in general, which is a persistent environmental problem in e.g. Thailand, being the major producer of farmed shrimp.[5,6] Adsorption mechanisms involve hydrogen bonding, π - π , and electrostatic interactions (Fig. 1). Our preliminary results suggested that the developed rPET/starch/PVOH adsorbent can be potentially used to remove antibiotics, which may be used in shrimp farms.

Our approach lies in the field of chemical recycling of PET and PEF. Since the formation of the hydrogels succeeded, the reaction conditions were preliminary optimized, and new blends with starch and poly(vinyl alcohol) (PVOH) were carried out. From the optimized conditions, the rPET-hydrogel was tested for anionic and cationic dye adsorption (Fig. 2; PET:starch:PVOH hydrogel: a) Dry, b) Water absorption, c) Congo red adsorption, d) Methylene blue adsorption.)[7] to see the possibility as an adsorbent in wastewater treatment application.

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On the Discrepancy between the Local and Average Electronic Structure in Hybrid Lead Halide Perovskites.

O. F. Dressler^{1,2}, S. Sabisch^{1,2*}, O. Ortikova^{1,2*}, M. Svyrydenko^{1,2*}, S. Elveren^{1*}, L. G. Feld^{1,2*}, L. Dubenska^{1,2*}, M. Kovalenko^{1,2*}

¹ETH Zürich, Department of Chemistry and Applied Biosciences, Vladimir-Prelog-Weg 1-5, Zürich CH-8093, Switzerland, ²Empa-Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, Dübendorf CH-8600, Switzerland

Colloidal semiconductor quantum dots (QDs) exhibit size-dependent optical and electronic properties, governed by quantum confinement effects. While optical spectroscopy provides insights into the average electronic structure, nuclear magnetic resonance (NMR) spectroscopy offers a complementary local perspective. In this study, we employ optical spectroscopy and ²⁰⁷Pb NMR spectroscopy to probe the confinement of three archetypical lead halide perovskites, namely CsPbBr₃, MAPbBr₃ and FAPbBr₃ QDs. All compositions show size dependent photoluminescence following the behaviour known from conventional QDs. NMR spectroscopy of CsPbBr₃ QDs confirms the size-dependent confinement seen for covalent semiconductor QDs where the average and local electronic structures both show signs of quantum confinement. On the other hand, FAPbBr₃ QDs lack a size-dependent chemical shift even though manifestations of confinement can be readily observed by optical spectroscopy. These findings provide direct experimental evidence for the previously proclaimed phonon-driven wavefunction localization in hybrid perovskites featuring dynamic cation disorder. This theory is further validated by MAPbBr₃ QDs which can be tuned between both modes of confinement by freezing out the dynamic disorder of the MA⁺ cation. By probing both the local and global electronic structure of QDs, this work reconsiders our understanding of quantum effects in lead halide perovskite QDs.

Non-invasive Quality Assessment of Melt-grown CsPbBr₃ by Nuclear Quadrupole Resonance Spectroscopy

L. Dubenska^{1,2}, S. Sabisch^{1,2*}, A. Kanak^{1,2*}, M. Kotyrba^{1,2*}, M. V. Kovalenko^{1,2*}

¹ETH Zürich, Department of Chemistry and Applied Biosciences, Vladimir-Prelog-Weg 1-5, Zürich CH-8093, Switzerland, ²Empa-Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, Dübendorf CH-8600, Switzerland

Lead halide perovskites (LHP) are promising material for direct hard radiation detection, a field that demands high-quality materials typically large melt grown crystals. While phase purity is confirmed using X-ray diffraction, quality assessments rely on optical microscopy and eventually on device performance — a process that is irreversible and requires full device fabrication. To address this problem, we establish nuclear quadrupole resonance (NQR) spectroscopy as a versatile, non-invasive technique for evaluating the quality of melt grown CsPbBr₃ ingots prior to the first device fabrication step. We show that, additionally to probing the local environment around a quadrupolar nucleus, NQR spectroscopy is inherently sensitive to crystal orientation and crystallinity. This is further supported by ab initio calculations. This approach enabled us to correlate key spectroscopic descriptors with macroscopic and microscopic structural features, to establish a robust evaluation of the crystal quality and a guided sample selection with regards to the crystallinity and crystal orientation. The use of modified resonators further allowed us to accommodate larger ingots, alleviated the need to remove them from the quartz ampule used during the growth and allowed for semi-automated special mapping of the spectroscopic descriptors across the ingots. We show that the removal of the impurities collected near the top of the ingot and subsequent recrystallization improve the homogeneity and overall crystallinity of the samples, highlighting the need for multiple purification steps. We also observed reorientation of the crystal domains along the ingot which is preserved after cutting. Our results deepen the understanding of both applied NQR spectroscopy and melt-growth processes of lead halide perovskites, paving the way for integrated quality control and innovative in situ applications.

Organic surface coating for high-voltage cathodes in LPSCI-based all-solid-state lithium metal batteries

A. Forster¹, J. Zhang^{2*}, A. Coskun^{1*}, M. El Kazzi^{2*}

¹University of Fribourg, Department of Chemistry, Chemin de Musée 9. 1700 Fribourg, ²PSI, Forschungsstrasse 111, 5232 Villigen

All-solid-state batteries (ASSBs) offer significant advantages over conventional lithium-ion batteries, such as improved safety, high energy density when paired with Li metal anode, and longer cycle life^[1]. However, ASSBs face multiple challenges, notably the interface with the cathode active material (CAM), which is prone to both physical and chemical degradation during cycling, especially when employing high-voltage CAMs such as $\text{LiNi}_{0.8}\text{Mn}_{0.1}\text{Co}_{0.1}\text{O}_2$ (NMC 811)^[2]. To address this issue, here, we introduced an organic anchoring strategy to stabilize the CAM surface and CAM-solid electrolyte interface using TFAAA. A weak acid-base interaction between the CAM and TFAAA creates a passivating layer as a highly competitive alternative to conventional sol-gel-applied inorganic coating, i.e., LiNbO_3 . Comparative electrochemical characterization of pristine, LNO-coated, and TFAAA-coated NMC811 verified the efficiency of the organic coating strategy. Furthermore, we observed significant suppression in the formation of Li_3PO_4 and $\text{P-S}_n\text{-P}$ species, indicating reduced decay of the LPSCI catholyte at the interface. These findings become apparent when studying the performance in CV and galvanostatic cycling (C/10) measurement. These show formation cycles and CEI formation, followed by stable cycling capacity over 125 cycles.

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Substitution of Formamidinium Cation into Rb-based Non-perovskite Phases Probed by Solid-state NMR Spectroscopy

U. Gunes¹, M. A. Hope^{1,2*}, Y. Zhang^{1*}, L. Zheng^{1*}, L. Pfeifer^{1*}, M. Grätzel^{1*}, L. Emsley^{1*}

¹Institut des Sciences et Ingénierie Chimiques, Ecole Polytechnique Fédérale de Lausanne, Lausanne 1015, Switzerland, ²Department of Chemistry, University of Warwick, Gibbet Hill Road, Coventry, CV4 7AL, UK

Hybrid lead-halide perovskite materials, including formamidinium lead iodide (FAPbI₃), are one of the promising candidates for next-generation solar cells. However, FAPbI₃ undergoes a spontaneous phase transition from the photoactive perovskite phase to a photoinactive non-perovskite phase, which significantly limits its application in commercial solar cells. This issue can be mitigated by including alkali metal cations such as cesium (Cs⁺) and rubidium (Rb⁺) in the perovskite synthesis. It has been shown by solid-state NMR spectroscopy that Rb⁺ does not substitute into the perovskite lattice in either single or double halide systems but instead forms a Rb-based non-perovskite phase. However, the mechanism by which Rb⁺ contributes to improved stability remains unclear.

Here, solid-state NMR spectroscopy is performed to reveal that FA⁺ cations incorporate into the Rb-based non-perovskite phases (FA_xRb_{1-x}Pb₂Br₅ and δ -FA_xRb_{1-x}PbI₃) for both bromide and iodide perovskites. This incorporation is evidenced by ¹H-⁸⁷Rb heteronuclear correlation (HETCOR) experiments, distinct changes in ¹H and ⁸⁷Rb chemical shifts, and complete signal dephasing in the ⁸⁷Rb{¹H} rotational echo double resonance (REDOR) spectra. Moreover, the REDOR dephasing curves were simulated to quantify the amount of FA⁺ incorporated into the Rb-based non-perovskite phase. The results show that up to ~60% FA⁺ is incorporated in the bromide system and ~15% in the iodide system. [1]

Furthermore, photoluminescence (PL) measurements show an enhanced signal upon substitution of FA⁺ into non-perovskite phase, suggesting improved crystalline quality and reduced defect density. We propose that the enhanced power conversion efficiency and improved stability in FA-based perovskites synthesized with Rb salts result from the segregation of excess FA⁺ cations.

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Metal-like Transport Behavior in In-plane Oriented Conjugated Polymers

L. Heinzen¹, D. Tsokkou^{1*}, E. Röck^{1*}, S. Guchait^{2*}, B. Jismy^{3*}, V. Bouylout^{2*}, M. Brinkmann^{2*}, N. Leclerc^{3*}, O. Bardagot^{1,3*}, N. Banerji^{1*}

¹Department of Chemistry, Biochemistry and Pharmacy, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland, ²Charles Sadron, Institute, CNRS University of Strasbourg, UPR 22, 23 rue du Loess, Strasbourg Cedex 02, 67034, France, ³Institute of Chemistry and Processes for Energy Environment and Health, CNRS University of Strasbourg, UMR 7515, 25 rue de Bexquerel, Strasbourg Cedex 02, 67087, France

Organic mixed ionic-electronic conductors (OMIECs) show promising advantages such as their versatile processing conditions, synthetic tuneability and their flexible nature. Additionally, the ability of this materials to enable both ionic and electronic transport makes it well-suited to interface biology and electronic devices. [1] So far, the field of bioelectronics has largely focused on device fabrication and performance. However, a comprehensive understanding of OMIEC charge transport mechanisms is still lacking. The electronic charge transport primarily occurs along the π -conjugated backbone, while ions penetrate the bulk material, interacting with the polymer matrix. [2,3]

In this study we investigate PBT^{TTT}-⁸O films oriented by high-temperature rubbing to gain a deeper insight into the fundamental processes of both ionic and electronic transport. Combining electrochemical and molecular doping with in-situ terahertz spectroscopy, spectro-electrochemistry, and chronoamperometry, we investigate the materials oxidation behavior and intrinsic charge transport properties. Terahertz spectroscopy measures the intrinsic nanoscale conductivity and gives access to short-range mobility, which is not affected by grain boundaries or electrodes.

Our findings reveal high conductivities exceeding 1000 S/cm for electrochemically doped PBT^{TTT}-⁸O films, and over 2000 S/cm for molecularly doped ones. In addition, using temperature-dependent THz measurements, we unravel the transport mechanism in oriented PBT^{TTT}-⁸O, which follows a metal-like transport behavior instead of thermally activated hopping behavior seen in lower conductive polymers, confirming the significant effect of in-plane orientation on OMIEC charge transport.

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Living Polymerization of Levoglucosenone-Derived Enyne Monomers: Tunable Degradation Rates and Higher Glass Transition Temperatures

E. Jung¹, A. Rizzo^{2*}, H. Ryu^{1*}, M. Cho^{1*}, T. Choi^{1*}

¹Department of Materials, ETH Zürich, Zürich, 8093, Switzerland, ²Department of Chemistry, the State Key Laboratory of Synthetic Chemistry, The University of Hong Kong, Pokfulam Road, Hong Kong 999077, P. R. China

In response to the growing concern over plastic waste pollution, the development of sustainable polymers has become increasingly important. Hence, biomass-derived degradable polymers offer a promising solution. One such candidate is levoglucosenone, a readily accessible compound obtained through the pyrolysis of cellulose, which holds strong potential as a monomer for polymer synthesis. However, the metathesis polymerization of levoglucosenone-based monomers has posed challenges due to their low reactivity, often requiring a highly reactive but unstable ruthenium catalyst (C793). To address this issue, we incorporated a cascade functional group, which enabled controlled polymerization of levoglucosenone-derived enyne monomers using a commercially available third-generation Grubbs catalyst. This living polymerization process also allowed for the synthesis of block copolymers. Additionally, we achieved tunable degradation kinetics spanning over two orders of magnitude by modifying monomer structure. Remarkably, by adjusting structural features, we obtained polymers with elevated glass transition temperatures in the range of 152–198 °C.

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Unveiling Surface Chemistry of Ultrafast-Sintered LLZO Solid-State Electrolytes for High-Performance Li-Garnet Solid-State Batteries

M. Klimpel^{1,2}, H. Zhang^{1,2*}, K. Wiecek^{3*}, R. Dubey^{1,2*}, F. Okur^{1,2*}, J. Michler^{3*}, L. Jeurgens^{4*}, D. Chernyshov^{5*}, W. van Beek^{5*}, K. Kravchyk^{1,2*}, M. Kovalenko^{1,2*}

¹Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ²Laboratory for Thin Films and Photovoltaics, Empa – Swiss Federal Laboratories for Materials Science and Technology, ³Laboratory for Mechanics of Materials and Nanostructures, Empa - Swiss Federal Laboratories for Materials Science and Technology, ⁴Laboratory for Joining Technologies & Corrosion, Empa - Swiss Federal Laboratories for Materials Science and Technology, ⁵Swiss-Norwegian Beamlines, European Synchrotron Radiation Facility

Ultrafast (UF) sintering emerges as a game-changing sintering methodology for fabricating $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO) solid-state electrolytes, representing a pivotal stride toward the advancement and prospective commercialization of Li-garnet solid-state batteries.^[1, 2] Despite its widespread use in the fabrication of LLZO ceramics, the chemical composition of the UF-sintered LLZO surface remains largely unexplored. This study presents an in-depth analysis of the surface chemistry of UF-sintered LLZO using comprehensive techniques, including depth-profiling X-ray photoelectron spectroscopy (XPS) and focused-ion-beam time-of-flight secondary ion mass spectroscopy (FIB-TOF-SIMS). Our investigation uncovers a striking difference between the surface of UF-sintered and conventionally-sintered LLZO, revealing a predominant surface contamination by Li_2O up to ca. 40 nm depth in the case of UF processing.^[3] Comparative synchrotron X-ray diffraction data during UF and conventional sintering elucidate the origin of surface contamination. We propose a viable solution to this issue through an additional heat-treatment (HT) step at 900 °C after UF sintering, as corroborated by XPS, and FIB-TOF-SIMS measurements. Furthermore, we present a comparative assessment of the electrochemical performance of Li/LLZO/Li symmetric cells based on UF-sintered LLZO pellets, both with and without the post-HT step, underscoring the pivotal role of an uncontaminated LLZO surface.

Figure 1. Surface composition of LLZO pellets after ultrafast sintering and post-thermal treatment, and electrochemical performance after each step.

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Designer Sulfonium-based Capping Ligands for Lead Halide Perovskite Nanocrystals

O. Kolomiets^{1,2}, A. Stelmakh^{1,2*}, A. Rajan^{1,2*}, S. Sabisch^{1,2*}, G. Rainò^{1,2*}, A. Baumketner^{3*}, M. Kovalenko^{1,2*},
M. Bodnarchuk^{1,2*}

¹Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir Prelog Weg 1, CH-8093 Zürich, Switzerland, ²Laboratory for Thin Films and Photovoltaics, Empa – Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland, ³Institute for Condensed Matter Physics, National Academy of Sciences of Ukraine, 1 Svientsitsky Str, Lviv, 79011, Ukraine

Lead halide perovskite nanocrystals (LHP NCs) exhibit instability due to the dynamic and labile nature of both their inorganic core and the organic-inorganic interface, adversely impacting their optical and electronic properties [1]. The quest for novel capping ligands has not stopped; rather, contrary [2], given the ever-expanding expectations for LHP NCs' deployment as classical and quantum light sources [3, 4]. We design a structurally diverse library of long-chain trialkylsulfonium ligands that provide robust surface passivation of CsPbBr₃ and MAPbBr₃ NCs, achieving photoluminescence quantum yields exceeding 90%. Classical force-field molecular dynamics simulations assess the trialkylsulfonium ligand head-group as a close analogue of a ubiquitous quaternary ammonium head-group regarding its binding to the perovskite surface. Conformational flexibility emerged as the dominant factor governing binding strength when comparing trialkylsulfonium ligands varying in the number and position of long alkyl chains. Guided by this fundamental understanding, we designed sulfonium-based zwitterionic ligands that form robust colloids with a suppressed blinking rate (on-time fraction ~85%) and high single-photon purity ($g^2(0) = 0.12$). Furthermore, applying “entropic” sulfonium ligands facilitates the stabilization of highly concentrated NC colloids (up to 1.1 g of inorganic mass per mL). These findings benchmark sulfonium-based ligands as practically applicable for diverse applications of LHP NCs.

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Thermally Evaporated Cesium Lead Halide Perovskites: From Structural Control to Optical Gain Applications

Y. Kominko^{1,2}, S. Yakunin^{1,2*}, M. Kovalenko^{1,2*}

¹Institute of Inorganic Chemistry, Department of Chemistry and Applied Bioscience, ETH Zürich, CH-8093 Zürich, Switzerland, ²Laboratory for Thin Films and Photovoltaics, Empa – Swiss Federal Laboratories for Materials Science and Technology, CH-8600 Dübendorf, Switzerland

Lead halide perovskites (LHPs) have attracted immense attention *via* the combination of their exceptional optoelectronic properties (high quantum efficiency, spectral tunability, large carrier diffusion length, high light absorption coefficient, long carrier lifetimes, narrow emission line width, good defect tolerance).^[1] Considering their advantages, LHPs are prospective materials various applications. However, in compact films, insulating ligands often limit heat and charge transport. Improving the heat management, for example, by removing ligands, can significantly improve the operational stability at high excitation densities required for laser devices.

This study presents the synthesis, structural characterization, and stable high optical gain of ligand-free nanocrystalline thin films obtained through single-source thermal evaporation of CsPbX₃ (X = Cl, Br).^[2] A slow post-deposition crystallization process under nitrogen yields compact, smooth, and optically uniform thin films with nanocrystalline grains with weakly confined optical features and pronounced excitonic resonances. The films show composition-tunable, low-threshold amplified spontaneous emission with a high net modal gain. Surpassing 5 hours of continuous operation under ambient conditions with merely ~8% degradation, the resulting films show great potential for the development of lasers and novel tunable optical amplifiers.

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Reinforcing Protein-Based Materials with Amyloid Nanofibrils for Sustainable Applications

A. Koptelova¹, F. Stellacci^{1*}, T. Abitbol^{1*}

¹EPFL

In the pursuit of sustainable materials, proteins offer promising potential due to their film-forming abilities, biodegradability, and bio-based origin.^{[1],[2]} Among them, whey protein – a by-product of the cheese-making industry – and soy protein – recoverable from by-products of soymilk and tofu production – have garnered attention for their capacity to form stable structures under specific conditions.^{[3],[4]} When exposed to low pH and elevated temperatures, proteins can self-assemble into amyloid nanofibrils, which are rich in β -sheet structures and exhibit enhanced mechanical and barrier properties.^[5]

In this work, we demonstrate how amyloid fibrils derived from whey and soy proteins can be used as nanoscale reinforcement agents in protein-based matrices. These protein–protein composites exhibit improved mechanical stability and moisture resistance, addressing key limitations of protein-based films for industrial applications such as food packaging. In this work we produce films from these protein–fibril composites and show that their properties can be tuned by varying the fibril content.

Our findings contribute to the development of fully bio-based and potentially compostable materials. Future work will focus on constructing multilayer systems entirely from protein-based components to enhance performance while maintaining recyclability and environmental compatibility.

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PFAS-free capacity boosters for energy dense redox flow batteries

J. Lorenzetti^{1,2}, C. Kupferschmid^{1*}, D. Reber^{1*}

¹Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland, ²École Polytechnique Fédérale de Lausanne, Institut des Matériaux, 1015 Lausanne, Switzerland

The low energy density of redox flow batteries can be mitigated by incorporating solid capacity boosters in the electrolyte tanks. A redox mediator in solution (electrolyte) is charged/discharged in the electrochemical cell and pumped into the tank where it reacts chemically with the booster (solid electrode material). If this reaction is reasonably fast, the energy density of flow batteries can be improved manyfold due to the much higher charge storage capacity of solid electrode materials compared to dissolved active species. For example, lithium iron phosphate (LFP) was shown to be a suitable capacity booster in combination with ferrocyanide as a redox mediator. Until now, polyvinylidene fluoride (PVDF) dissolved in *N*-Methylpyrrolidone (NMP) has been used as a binder in the manufacturing of booster pellets. Amid growing concerns and tightening regulations surrounding PFAS compounds, we extruded LFP pellets with polycaprolactone (PCL), a biodegradable binder, dissolved in more benign *N,N*-Dimethylformamide (DMF), and screened their reaction rates using on-line UV-Vis spectroscopy. By replacing PVDF with PCL, the reaction rate between LFP and ferricyanide increased three-fold, arguably due to the lower hydrophobicity of PCL and improved interaction between the mediator solution and the boosters. We demonstrate that using non-fluorinated binders improves the performance of LFP pellets while preserving their structural integrity, paving the way for more sustainable, PFAS-free solid boosters. Importantly, we also show that the positioning of the booster pellets directly in the electrolyte path is of great importance for improved reaction rates and material utilization, highlighting mass transport as a limiting factor in flow batteries enhanced by solid boosters.

Engineering Liquid Crystalline Photoresists for Xolography Applications

K. D. Milanov¹, F. Trigka^{1*}, M. Lerch^{1*}

¹Stratingh Institute for Chemistry, University of Groningen, Nijenborgh 7, 9747 AG, Groningen, The Netherlands

Polymeric Liquid Crystalline (LC) materials are tunable stimuli-responsive materials.^[1] Maximization of the stimuli-response can be achieved by use of Liquid Crystalline Elastomers (LCEs) making monolithic LCEs promising materials for multifunctional applications in sensing, load-bearing, and adaptive systems.^[1-2] Volumetric Additive Manufacturing (AM) methods such as Two-Photon Polymerization Direct Laser Writing (TPP-DLW) and Computed Axial Lithography (CAL) rely on nonlinear photoresists, constraining resolution and fabrication speed.^[3] Xolography—a novel volumetric AM approach using dual-beam light field projection—circumvents these limitations by enabling sectional image generation within a resin volume, and moving away from sequential AM.^[3] Despite its potential, the application of xolography to LCEs is hindered by the stringent optical and thermal requirements of suitable photoresists. Here, we report the development of LC monomer formulations optimized for xolography. By tuning crosslinker content and rational design of mesogenic units, we controlled transition temperatures (T_{NI} s). Mixture photopolymerization was enhanced by employing thiol-ene chemistry. Partial success was achieved in improving optical transparency as revealed by Polarized Optical Microscopy (POM) with an increase in polydomain formation upon addition of 1 w% *N,N',N''*-(benzene-1,3,5-triyl)tris(2,2-dimethylpropanamide). Our results establish a foundation for next-generation xolography photoresist formulations tailored to different LC functional classes. This work opens avenues to further enhance the optical properties of the photoresist and integrate all key requirements—transition temperatures, photopolymerization, and transparency—into a single functional system.

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Self-Degrading Chromogenic Polymer

O. Mondal¹, G. Formon^{1*}, S. Rowan^{2*}, C. Weder^{1*}

¹Adolphe Merkle Institute, University of Fribourg, Fribourg, Switzerland, ²University of Chicago, USA

Mechanical and structural degradation can cause a loss of functionality in polymers, but this often goes unnoticed during the product's useful life, when aging occurs.¹ Consequently, there is a growing interest in developing polymers that visually indicate defects² as well as the aging process.³ On the other hand, the possibility to develop polymers that degrade in a controlled manner is useful for applications ranging from biomedicine to environmentally degradable plastics. Dynamic covalent chemistry has revolutionized polymer design by enabling reversible bond formation and dissociation. By modifying the composition of different dynamic covalent networks, a wide range of functions, including self-healing and recycling can be realized.⁴ Here, we report a self-degrading polyurethane, whose degradation is accompanied by a chromogenic response that enables the real-time detection of aging. The new polymer contains dynamic thia-Michael bonds, which facilitate degradation and trigger a visible color change as the polymer ages. To achieve this, we designed conjugated dyes that act as Michael acceptors and can react with thiols to form colorless Thia-Michael adducts. Monomers based on this design were covalently incorporated into the backbone of a thermoplastic polyurethane elastomer. As the thia-Michael bond formation is reversed, the polymer's molecular weight is reduced and the dyes are restored, leading to a chromogenic response that visibly signals the aging process.

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Tuning Charge Transfer in Novel NDI–Pyrene Paracyclophanes: Role of Interchromophore Distance and Linker Structure

C. Negrete-Vergara¹, V. Slama^{2*}, E. Zyaee^{3*}, G. Graf^{1*}, S. Decurtins^{1*}, R. Häner^{1*}, H. M. Frey^{3*}, T. Feurer^{3*}, U. Röthlisberger^{2*}, S. X. Liu^{1*}

¹Department of Chemistry, Biochemistry and Pharmaceutical Sciences, W. Inäbnit Laboratory for Molecular Quantum Materials and WSS-Research Center for Molecular Quantum Systems, University of Bern. Freiestrasse 3, Bern CH-3012, Switzerland, ²Laboratory of Computational Chemistry and Biochemistry, Institute of Chemical Sciences and Engineering, EPFL, Lausanne, Switzerland., ³Institute of Applied Physics, University of Bern, Sidlerstrasse 5, Bern CH-3012, Switzerland

Understanding charge transfer (CT) and charge delocalization phenomena is indispensable for manufacturing molecular devices. Traditional approaches often rely on covalently linked donor-acceptor (D-A) systems via π -conjugated bridges, but these usually suffer from solubility and aggregation issues. Recently, non-covalent through-space CT systems have gained attention, offering a more tunable approach by spatially arranging D and A units using flexible linkers[1]. Among these, paracyclophane (PCP) scaffolds are particularly promising due to their rigid yet customizable structure that promotes close D-A stacking. Naphthalene diimide (NDI), known for its electron-deficient character and n-type semiconducting properties, has been widely employed as an acceptor in such systems[1]. Despite notable advances in supramolecular polymers and single cocrystals based on NDI and pyrene[2,3], a comprehensive understanding of through-space CT dynamics in PCP ensembles remains limited. To address this gap, this study presents novel PCPs combining pyrene (donor) and NDI (acceptor) units linked by varied bridges like phenyl and adamantyl groups, as shown in the figure below. Their structural characterization revealed that the linker type and interchromophore distance significantly influence the π - π stacking interaction and, consequently, their photophysical properties, as evidenced by a new band appearing between 500-600 nm in the optical spectra. Time-resolved transient absorption spectroscopy combined with DFT calculations offers valuable insights into the properties and photophysical behavior, offering a deeper understanding of through-space CT mechanisms in these novel PCP-based molecular structures.

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From waste to value: extraction of phytin from oilseed presscakeG. Panzarasa^{1,2}¹Wood Materials Science, ETH Zurich, Laura-Hezner-Weg 7, 8093 Zurich (Switzerland), ²NeoChemurgy GmbH

Phytin, the calcium and magnesium salt of *myo*-inositol hexaphosphate, is a form of organic phosphorus widespread in vegetables and especially in their seeds [1]. The seeds of oil crops, such as sunflower and rapeseed/canola, are especially rich in phytin, which remains in the presscake after the extraction of oil. The presscake is also rich in proteins and other nutrients, and as such is commonly used as cattlefeed. However, the metal-chelating properties of phytin make it a potent antinutrient, requiring the cattlefeed to be supplemented with minerals.

Common procedures for phytin extraction involve the use of mineral acids, which affect the nutritional profile of the residue and could result in the generation of unwanted by-products.

A convenient, food-safe method to extract phytin from rapeseed presscake was developed [2], allowing the residue to be used as cattlefeed. The process makes use of an organic acid-based aqueous pH buffer to ensure a mild but fast extraction of phytin, which can then be precipitated as a solid by changing the solution pH, or further processed e.g. into phytic acid, which in turn can be used to produce high-added value products such as bio-based fire-retardants.

Phytin and phytic acid are not only valuable industrial products in the broad biorefinery concept, they prove their worth also for more fundamental applications in materials science.

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RAdiolanthanide Production In Core (RAPIC)

S. Pasolini^{1,2}, P. Steinegger^{1,2*}, Z. Talip^{1*}, E. A. Maugeri^{1*}

¹PSI, ²ETHZ

Radiolanthanides, such as ¹⁷⁷Lu and more recently ¹⁶¹Tb have significant potential in targeted radionuclide therapy for cancer treatment. The RAPIC project proposes an innovative method for their production *via* neutron irradiation of targets with embedded lanthanides enriched in a certain isotope (e.g., ¹⁷⁶Yb and ¹⁶⁰Gd) within the core of the Nuclear Power Plant Gösgen (KKG). The employment of the existing Aeroball core monitoring system (AMS) for neutron flux measurements, would allow for the production of these radionuclides. Currently, these are exclusively produced using nuclear research reactors. Hence, this project is concerned with the production and casting of well-defined spheres (i.e., following the size and mechanical constraints given by the AMS) of intermetallic compounds of the targeted lanthanide element and platinoid metals through a high-temperature, hydrogen-mediated reduction process known as coupled reduction [1].

Ongoing efforts focus on optimizing the synthesis parameters, such as the lanthanide-to-platinoid ratio, processing temperatures, holding times, and annealing conditions. These optimization studies aim to enhance mechanical integrity and irradiation stability. The characterization of the produced materials involves performing iteratively X-ray diffraction for phase identification and scanning electron microscopy in combination with energy-dispersive X-ray spectroscopy for microstructural and compositional analysis. Shaping and mechanical tests will be performed to evaluate the hardness, toughness, and deformation resistance under conditions mimicking the reactor core injection using the AMS. The most promising products will then undergo neutron irradiation tests at the Swiss Spallation Neutron Source SINQ at PSI (i.e., similar neutron flux as encountered at KKG) to evaluate the irradiation stability and the production yield. In a final step, a suitable chemical separation and purification strategy will be devised in order to obtain high-purity, non-carrier-added radiolanthanides for medical applications. These efforts will ultimately enable a reliable and scalable production pathway for ¹⁷⁷Lu and ¹⁶¹Tb using existing installations in a commercial nuclear power plant, potentially improving the overall availability of these radionuclides for nuclear medicine in Switzerland and beyond.

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Towards the development of an electric organ to power artificial muscles

C. Pierucci^{1,2}, M. Rojas Cessa^{2*}, N. Zahnd^{1*}, M. Mayer^{1,2*}, A. Ianiro^{1,2*}

¹Adolphe Merkle Institute, University of Fribourg, Chemin des Verdiers 4, Fribourg 1700, Switzerland, ²Swiss National Center for Competence in Research (NCCR) Bio-inspired Materials, University of Fribourg, Chemin des Verdiers 4, Fribourg 1700, Switzerland

Fish such as Torpedo rays and Electric eels have evolved the ability to transform metabolic energy into powerful electrical discharges. Inspired by this natural phenomenon, we are developing implantable artificial electric organs capable of powering active devices such as artificial muscles and pacemakers.

We are currently exploring three main strategies:

- constructing reverse electrodialysis (RED) systems using hydrogels¹,
- utilizing commercial proton exchange membranes like Nafion²,
- and fabricating ultrathin membranes through the self-assembly of amphiphilic block copolymers (BCPs)³.

Preliminary results show that all three approaches can successfully generate compact and efficient artificial electric organs at a small scale. As we continue refining these systems, we believe they could significantly impact future technologies in active prosthetics, soft robotics, and energy-autonomous biomedical devices.

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Understanding the Role of the Acid/Base Sites in the Supported Cu/ZnO Catalysts for the CO₂ hydrogenation to Methanol

I. M. Popa¹, C. Pischetola^{1*}, L. Artiglia^{1*}, V. Sushkevich^{1*}, J. A. van Bokhoven^{1,2*}

¹Center for Energy and Environmental Sciences, Paul Scherrer Institute, Forschungsstrasse 111, 5232 Villigen, Switzerland, ²Institute for Chemical and Bioengineering, ETH Zurich, Vladimir-Prelog-Weg 1, 8093 Zurich, Switzerland

Closing the anthropogenic carbon cycle is one of the biggest challenges of the 21st century. A promising strategy is the conversion of CO₂ into value-added chemicals, such as methanol. Industrially, the selective hydrogenation of CO₂ has been performed over the heterogenous catalyst Cu/ZnO/Al₂O₃ (CZA) for the past few decades, yet the precise reaction mechanism and the nature of active sites under catalytic conditions (50-100 bar and 200-300 °C) remains highly debated. A consensus has been reached about the Cu/ZnO synergy, but the exact nature of this effect remains uncertain due to the challenge of collecting characterization data at elevated pressures. Recent works have attempted to close this pressure gap, predominantly focusing on the Cu/ZnO interaction and largely neglecting the role of the Al₂O₃.^[1] Current hypotheses regarding the role of this oxide include its involvement in the CO₂ activation, and the possibility of the surface OH-groups being important actors in the catalytic cycle.^[1-2]

This work aims to investigate the role of the acid/base sites of the supporting material in the CO₂ activation and elucidate the selective hydrogenation mechanism. The CO₂ activation mechanism (bending, repartition of charges, electron transfer or hydride transfer) on acid/base sites of different strengths or nature (Lewis *versus* Brønsted) and understanding how these sites affect the key intermediates and overall reaction mechanism are some of the open questions we set out to answer through this project.

For this purpose, several metal oxides with different acidities (MgO, SiO₂, ZrO₂, Al₂O₃ and Ga₂O₃) are synthesized through precipitation and impregnated with 10 w% Cu and 5 w% Zn (CuZn/oxide). Their structures are confirmed by means of X-Ray diffraction (XRD) and the surface species are investigated using X-Ray photoelectron spectroscopy (XPS). Scanning electron microscopy coupled with energy-dispersive X-Ray (SEM-EDX) reveals surface etching of the more basic substrates upon impregnation. The acid and basic sites are quantified through NH₃ and CO₂-temperature programmed desorption (TPD), respectively, while the nature of these sites is revealed through pyridine and CO₂ Fourier-Transform infrared (FTIR) probing. Different CO₂-species are detected, including mono- and bidentate bound carbonates, bridged carbonates and hydrogencarbonates, which might act as the precursors for the formate intermediates.^[2] Moreover, the deposition of Cu and Zn is shown to affect the nature of the acid/base sites and to significantly decrease the surface area of the supports, as quantified through N₂-physisorption. The CuZn/oxide materials are then used as catalysts in the CO₂ hydrogenation to methanol at 200-300 °C and 15-30 bar under a stoichiometric CO₂:H₂ 1:3 flow.

Our results show that the acid/base properties of the support play an important role in the CO₂ activation which is crucial for the rational design of novel catalysts.

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Exploiting the LDH Memory Effect in the Carbon Dioxide to Methanol Conversion

I. M. Popa¹, G. Carja^{2*}, J. A. van Bokhoven^{1,3*}, F. Krumeich^{4*}, C. Pischetola^{1*}, L. Artiglia^{1*}

¹Center for Energy and Environmental Sciences, Paul Scherrer Institute, Forschungsstrasse 111, 5232 Villigen, Switzerland, ²Department of Chemical Engineering, Faculty of Chemical Engineering and Environmental Protection Technical University "Gheorghe Asachi" of Iasi Bd. D. Mangeron no 71, Iasi 700050, Romania, ³Institute for Chemical and Bioengineering, ETH Zurich, Vladimir-Prelog-Weg 1, 8093 Zurich, Switzerland, ⁴Department of Chemistry and Applied Biosciences, Institute of Inorganic Chemistry, ETH Zürich, CH-8093 Zürich, Switzerland

The conversion of carbon dioxide into platform chemicals such as methanol using copper-zinc oxide-alumina (CZA) catalysts is one of the most studied reactions of the past decade.^[1] Recent research has focused on devising modified CuZnAl catalytic systems where the synergistic effect between zinc-copper species can stabilize Cu active nanospecies. A variety of materials have been tested as catalyst precursors for this reaction, including layered double hydroxides (LDHs). LDHs are particularly appealing due to their structural 'memory effect', which enables the layered structure to be restored after destruction caused by calcination.^[2] This effect can be exploited to create novel properties in LDH materials, the catalytic potential of which has yet to be fully exploited.

In this work, a family of novel catalysts was developed through successive reconstructions of CuZnAl and CuZnMgAl LDH in Cu(CH₃COO)₂ aqueous solution, and thoroughly characterized by means of X-ray diffraction, electron microscopy and photoelectron spectroscopy. The repeated cycles of calcination, followed by the reconstruction process, led to the formation of heterostructures based on the recovered LDH structure with CuO nanoparticles (NPs < 5 nm) embedded within the LDH platelets. Each calcination-reconstruction cycle led to increasingly smaller and more monodisperse CuO NPs. The reductive activation of the LDH material induced the formation of Cu and ZnO NPs with larger Cu/ZnO interface after each consecutive calcination-reconstruction cycle. This Cu/ZnO synergy allowed over 60% methanol selectivity at 250°C and 30 bar during CO₂-to-methanol conversion. These results offer key insights for designing more efficient catalytic systems for future CO₂-to-methanol synthesis.^[3]

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Implementation of Safe and Sustainable by Design (SSbD) Vision for Materials Development: Case Study with Flame Retardant Vitrimers

R. Reis¹, A. Sekar^{2*}, C. Hervieu^{2*}, S. Gaan^{2*}, S. Gaan^{2*}, K. J. Groh^{1*}, K. J. Groh^{1*}

¹Department of Environmental Toxicology, Eawag, Swiss Federal Institute of Aquatic Science and Technology, Ueberlandstrasse 133, 8600 Dübendorf, Switzerland, ²Additives and Chemistry, Advanced Fibers Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, Lerchenfeldstrasse 5, 9014 St. Gallen, Switzerland

The Safe and Sustainable by Design (SSbD) framework, launched in 2022 under the European Green Deal, is gaining traction as a guiding concept for aligning material innovation with environmental and health protection goals. To facilitate wider adoption of SSbD principles among material scientists, practical demonstrations of tailored approaches are needed—especially those that support an early integration of safety considerations into the research & development process [1]. However, most SSbD case studies to date have focused on existing chemicals, with limited application during molecular design or material development [2]. Consequently, there is a need for further research into SSbD tools and smart workflows to enable efficient testing and informed decision-making at early design stages.

The study presented here implements an SSbD-guided workflow for iterative optimization of epoxy-based vitrimers. Due to incorporation of polyphosphonate structures into covalent adaptable networks, these materials can offer both the flame retardancy and thermomechanical reprocessability—properties that must be balanced against potential environmental impacts [3]. To this end, we apply a tiered testing strategy using fish cell- and embryo-based tests (OECD Test Guidelines 249 and 236, respectively) to assess the aquatic toxicity of monomers, cross-linkers, and leachates from these materials, aiming to understand the contribution of material formulation, curing processes, and reprocessing cycles to the observed toxicity. Combined with material properties and functionality assessment, generated toxicity data are then iteratively used to guide the subsequent steps toward material improvement.

This case study not only supports the development of high-performance, low-toxicity flame-retardant vitrimer materials, but also provides a broadly applicable demonstration of how the toxicity assessment can be meaningfully embedded into the material design process. We thus offer a model for interdisciplinary collaboration among chemists, material developers, and toxicologists. By sharing our experience, we hope to initiate a wider dialogue among the SCS material science community and encourage further SSbD-driven material innovation.

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Funktionalisierung von Silica-Oberflächen zur verbesserten Endothelzelladhäsion; Eine Grundlage für 3D-Modelle der Blut-Hirn-Schranke

K. Samietz¹, B. Brand^{1*}

¹Zürcher Hochschule für Angewandte Wissenschaften (ZHAW), Institut für Chemie und Biotechnologie

Die Blut-Hirn-Schranke (BBB) bildet eine essenzielle Barriere zwischen Blutkreislauf und zentralem Nervensystem und ist für die pharmakologische Forschung von grosser Bedeutung. Konventionelle 2D-Modelle der BBB stossen jedoch an ihre Grenzen, weshalb zunehmend physiologisch relevantere 3D-Modelle entwickelt werden. Diese Arbeit befasst sich mit der funktionellen Oberflächenmodifikation von additiv hergestellter, poröser Silicascheiben, die als Trägermaterial für ein zukünftiges 3D-BBB-Modell dienen sollen. Ziel war die Entwicklung eines Verfahrens zur Verbesserung der Adhäsion von Endothelzellen, insbesondere durch die Optimierung der (3-Aminopropyl)triethoxysilane (APTES)-basierten Silanisierung und anschliessender kovalenter Bindung von RGD-Peptiden.

Untersucht wurden verschiedene Funktionalisierungsprotokolle mittels DRIFTS, Kontaktwinkelmessung, Gassorptionsanalyse und Elementaranalyse. Dabei erwiesen sich insbesondere Trocknung und Oberflächenreinigung als entscheidend. DRIFTS-Spektren und Kontaktwinkelmessungen bestätigten eine erfolgreiche Oberflächenmodifikation. Aufgrund der geringen Silanolgruppen auf den Disks war deren direkte Analyse limitiert, konnte jedoch durch Experimente mit Silica-Gel und Objektträgern gestützt werden.

Zur weiteren Funktionalisierung wurde eine Methode zur kovalenten Anbindung von *p*-Phenylendiisothiocyanat (PDITC) entwickelt, um anschliessend RGD-Peptide zu koppeln. Der Nachweis der PDITC- sowie der Peptidbindung erfolgte über LC-MS, wobei für Letztere die Dansyl-Edman-Sequenzierung zum Einsatz kam.

Green Hydrogen Meets Biomass Upgrading: A Dual-Function PEC System Using Abundant Sb₂Se₃ and Copper

R. Schnyder¹, T. Moehl^{1*}, D. Tilley^{1*}

¹Department of Chemistry, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland

Photoelectrochemical water splitting using abundant, low-cost semiconductors is a promising method to produce green hydrogen from solar energy. Antimony selenide (Sb₂Se₃) is an emerging photocathode material with several advantages, including a small bandgap and high stability. However, it suffers from relatively low photovoltage, making it difficult to drive overall water splitting.

To facilitate hydrogen generation, the oxygen evolution reaction (OER) can be replaced with a simpler and more valuable oxidation reaction. One such reaction is the oxidation of the biomass-derived platform chemical 5-hydroxymethylfurfural (HMF) to 2,5-furandicarboxylic acid (FDCA), a key precursor for bio-based plastics.

In this project, Sb₂Se₃ was paired with abundant metallic copper as an HMF oxidation catalyst. Copper enables the oxidation of HMF to 5-hydroxymethyl-2-furancarboxylic acid (HMFCa) at potentials as low as 0.1 V vs. RHE in alkaline solution. However, the provided photovoltage must be limited to prevent self-oxidation of copper, making Sb₂Se₃ an ideal photocathode.

By optimizing copper electrodeposition conditions, it was possible to significantly enhance its surface area and the resulting current density for HMF oxidation. After a brief activation, the combined electrodes operated without external bias for over 1 hour, simultaneously producing hydrogen and HMFCa.

The results demonstrate the potential of combining Sb□Se□ and copper for efficient, bias-free photoelectrochemical conversion of sunlight and biomass-derived compounds. The integrated approach enables green hydrogen production while simultaneously generating value-added chemicals like HMFCa. Together, these features offer a sustainable route to fuels and bio-based materials using earth-abundant components.

Shedding Light on the Bulk and Surface Features of Alumina Polymorph combining TEM, IR and XRD

C. Sidhoum¹, C. Copéret^{1*}

¹Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir-Prelog Weg 1–5/10, CH-8093 Zürich

Aluminium oxide Al_2O_3 , and particularly its metastable phase gamma-alumina ($\gamma\text{-Al}_2\text{O}_3$), is widely used in various industrial applications, including as a support for heterogeneous catalysts, in pollutant adsorption, and as a ceramic coating. Nevertheless, a clear and comprehensive structural description of gamma-alumina ($\gamma\text{-Al}_2\text{O}_3$) remains challenging. Several structural models have been proposed, focusing primarily on the location of aluminum vacancies and the distribution of aluminum between octahedral and tetrahedral lattice sites [1].

In this context, we investigate two metastable phases of alumina—eta (η) and gamma (γ)—which, while structurally close, exhibit slight differences in acidity, making them suitable for comparative analysis. Using high-resolution transmission electron microscopy (HRTEM), we observed that needle-like $\gamma\text{-Al}_2\text{O}_3$ crystals exhibit the expected (100) and (110) facet orientations (Figure 1.A), whereas triangular $\eta\text{-Al}_2\text{O}_3$ crystals show an overrepresented (111) facet (Figure 1.B). These HRTEM findings align with subtle differences in the X-ray diffraction (XRD) patterns, where the (111) facet appears exclusively in $\eta\text{-Al}_2\text{O}_3$. Additional Fourier Transform Infrared (FTIR) spectroscopy (Figure 1.D) reveals significant intensity shifts between both phases, indicating variations in the surface aluminum coordination [2], consistent with the structural features observed via XRD and HRTEM. Further 2D NMR (^1H - ^1H and ^{27}Al - ^1H) measurements will support these observations and contribute to the development of a surface model for $\eta\text{-Al}_2\text{O}_3$, building on previous work from our group [3].

Through this study, we clarify the surface characteristics of both polymorphs to better understand the reactivity of metastable alumina phases as catalyst supports.

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Feasibility of Pyrochlore-type Iron(III) Hydroxy Fluorides as Cathode Materials in $\text{Li}_6\text{PS}_5\text{Cl}$ All-Solid-State Batteries

J. Šivavec^{1,2}, J. F. Baumgärtner^{1,2*}, D. C. Stoian^{3*}, M. Klimpel^{1,2*}, W. v. Beek^{3*}, K. V. Kravchyk^{1,2*}, M. V. Kovalenko^{1,2*}

¹Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir-Prelog-Weg 1, CH-8093 Zürich, Switzerland, ²Laboratory for Thin Films and Photovoltaics, Empa – Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland, ³Swiss-Norwegian Beamlines, European Synchrotron Radiation Facility, Grenoble 38000, France

The argyrodite-type $\text{Li}_6\text{PS}_5\text{Cl}$ (LPSCl) is considered one of the most promising solid-state electrolytes for practical applications. However, it must be paired with a suitable cathode material. Due to concerning projections of Ni and Co shortages, which are essential elements in most state-of-the-art cathodes, the exploration of novel, cost-efficient materials is imperative.² Our work explores pyrochlore-type iron(III) hydroxy fluorides (Pyr-IHF) as a suitable candidate due to abundant reserves of its constituent elements and their excellent electrochemical performance in liquid electrolyte systems.³

Electrochemical measurements of Pyr-IHF/LPSCl cells show that the cathodes can deliver a high initial charge capacity of 172 mAh g^{-1} at 0.1 C , with reasonable capacity retention of *ca.* 65 % after 50 cycles.⁴ A detailed analysis of the system, employing energy dispersive X-ray spectroscopy and X-ray absorption spectroscopy, reveals a pronounced redox reaction between Pyr-IHF and LPSCl, resulting in significant capacity contributions from sulphur redox during electrochemical cycling.

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Improving local antibiotic therapy through the study of interactions and release mechanisms between CaSO₄ carriers and antibiotics

D. Stefanita^{1,2}, D. Terebenec^{2*}, P. Wahl^{3,4*}, A. Neels^{2,5*}

¹Department of Chemistry, University of Fribourg, Fribourg, ²Center for X-ray Analytics, Empa, Swiss Federal Laboratories for Materials Science and Technology, ³Faculty of Medicine, University of Bern, ⁴Department of Biomedical Engineering, University of Basel, ⁵Department of Chemistry, University of Fribourg

Treating infections in orthopaedic and trauma surgery remains a significant challenge, requiring novel and effective therapeutic solutions.¹ Local antibiotic therapy enables the delivery of antibiotics directly to bone and joint infections, while minimizing systemic toxicity.² Calcium sulfate (CaSO₄) has emerged as a promising osteoconductive carrier for antibiotics, such as vancomycin² and ceftriaxone,³ and tobramycin⁴ due to its biocompatibility and biodegradable properties. This study aims to investigate the molecular interactions and controlled uptake mechanisms of antibiotic-loaded CaSO₄ carriers. The research applies a comprehensive analytical approach, utilizing powder X-ray diffraction (PXRD) as the primary technique for in-situ kinetic studies of drug-carrier interactions at the molecular level. PXRD was used to track in real-time the polymorphic transition from hemihydrate to gypsum,⁵ which depends on the hydration state of the CaSO₄ matrix loaded with various antibiotics. Kinetic analysis revealed distinct transformation rates: $0.040 \pm 0.015 \text{ min}^{-1}$ for CaSO₄_Ceftriaxone, $0.045 \pm 0.005 \text{ min}^{-1}$ for CaSO₄_Vancomycin, and $0.002 \pm 5 \times 10^{-4} \text{ min}^{-1}$ for CaSO₄_Tobramycin. Additionally, thermogravimetric analysis (TGA) reveals information on the hydration state and thermal stability of the Ca-Ceftriaxone complex, while pH analysis provides insights into the chemical nature of these compounds in solutions.

These studies provide critical insights into hydration state dependent release kinetics and polymorphic transition⁵ in CaSO₄-antibiotic systems. Understanding of drug-carrier interactions is supporting the advancement of local antibiotic delivery, improving infection management and clinical outcomes in orthopaedic and trauma surgery.

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Hydrogenative Depolymerization of Polystyrene Initiated by KH/C

P. Tian¹, A. Fedorov^{1*}

¹Department of Mechanical and Process Engineering, ETH Zürich, Switzerland

Polystyrene (PS) is a commodity plastic with an annual production of millions of tons. Despite this considerable scale, the chemical recycling of PS waste remains underdeveloped, with only about 1% of PS waste being recycled.^[1] Therefore, identifying novel approaches for the chemical recycling of PS, such as transforming PS waste into valuable chemicals, is crucial. In this context, transition-metal-catalyzed hydrogenolysis of plastic waste is regarded as an emerging valorization technology.^[2-3]

We have recently reported that a catalytic amount of carbon-supported potassium hydride (KH/C) enables the hydrodemethylation (HDM) of toluene to benzene at 250 °C under 50-80 bar of H₂.^[4] The mechanism of this C(sp²)-C(sp³) bond cleavage of toluene supposedly involves hydrogen radicals, generated from H₂ in situ, that act as a radical chain transfer species. Here, we have applied the [KH/C + H₂] methodology to a slurry of PS in dodecane and uncovered a selective hydrogenative depolymerization of various grades of PS, including consumer-grade PS, which proceeds at notably milder conditions relative to the above-mentioned HDM of toluene. Specifically, using a low loading of KH/C (1 mol %), PS is converted fully into a ca. 6 : 1 : 1 mixture of ethylbenzene, toluene, and cumene (Figure 1). Compared to alternative state-of-the-art hydrogenolysis approaches,^[2-3] our methodology is more energy- and cost-efficient as it operates at low temperature and H₂ pressure (160 °C, 2-10 bar). The reaction time can be as short as one hour, and the KH/C initiator can be separated from the liquid product mixture by filtration and recycled. The present results demonstrate a practical pathway to the chemical recycling of PS that uses a cheap and recyclable initiator based on an earth-abundant metal.^[5]

Figure 1. a) Products of the hydrogenative depolymerization of PS and reaction conditions. b) PS materials used for the reaction. c) The depolymerization tests of various grades of PS (180 °C, 10 bar H₂) and d) recyclability studies with **1-r** (220 °C, 30 bar H₂) in dodecane.

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High dielectric permittivity polysiloxanes for solvent-free industrial processing

J. Wolf^{1,2}, P. M. Danner^{1,2*}, D. M. Opris^{1,2*}

¹EMPA – Swiss Federal Laboratories for Materials Science and Technology, Functional Polymers Laboratory, Überlandstrasse 129, 8600 Dübendorf, Switzerland, ²ETH Zürich, Departement of Materials, Vladimir-Prelog-Weg 5, 8093 Zürich, Switzerland

High-dielectric-permittivity polysiloxanes hold great potential for applications in batteries and dielectric elastomer transducers (DET).[1,2] Despite their promising performance in DET, large-scale production remains unestablished due to processing challenges. These materials tend to dewet on standard industrial substrates like stainless steel, and their thiol-ene cross-linking is incompatible with platinum catalysts commonly used for polydimethylsiloxane thermal curing. This work presents a composite of cyano-propyl-functionalized polysiloxane and Elastosil designed to enhance processability while increasing dielectric permittivity. We successfully produced this ink at a 40-gram scale and utilized epoxy-based curing to eliminate catalyst poisoning. The composite's mechanical and electrical properties were systematically evaluated, and actuator prototypes were fabricated and tested. Our results demonstrate improved manufacturability and performance, advancing high-permittivity polysiloxanes toward industrial integration.

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Light Responsive Peptide-Chromophore Conjugates

J. F. Woods¹, H. Wennemers^{1*}

¹Laboratory of Organic Chemistry, ETH Zürich, Vladimir-Prelog-Weg, Zürich, 8093, Switzerland

Self-assembly can yield complex molecular architectures from simple molecules. The formation process of such extended supramolecular assemblies can be delicate. Even slight alteration of conditions or seemingly simple modifications to a molecular building block can lead to drastically different results.¹ A major challenge is not only to create robust assemblies, but also to control them with external stimuli such as temperature or light.

Our group has reported the self-assembly of oligoproline-chromophore conjugates into several morphologies, including fibers, ribbons, nanosheets and woven frameworks.²⁻⁴ Installation of anthracene as the chromophore within these conjugates also allows for self-assembly into one-dimensional (1D) fibers from THF/H₂O mixtures. Optical responses vary according to the amount of water present in solution, notably affecting the morphologies in terms of thickness and length as the proportion of water increases from 70 to 90%. When irradiated with blue light, photocyclization occurs and prompts collapse of the fibers, demonstrating the responsiveness of this system to stimulus.

Structure of an oligoproline functionalized with anthracene moieties, left, that self-assembles into 1D fibers as observed from TEM, middle, and disassemble upon irradiation, right.

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Buffer Layer Interface Repair Engineering for Artificial Photosynthesis of Antimony Selenide

Z. Zhang¹, T. Moehl^{1*}, T. Moehl^{1*}, D. Tilley^{1*}

¹Department of Chemistry, University of Zurich, Winterthurerstrasse 190, CH-8057 Zurich

With the growing demand for clean energy technologies, photoelectrochemical (PEC) systems have emerged as a promising approach for sustainable energy conversion. Antimony selenide (Sb_2Se_3) is a highly investigated material due to its excellent photovoltaic properties; however, its application in PEC water splitting is still limited by interfacial charge recombination and inefficient carrier transport. To address these challenges, this study presents a novel strategy for developing cadmium-free In_2S_3 buffer layers with interface repair engineering, aiming to enhance the PEC performance of semiconductor heterojunctions. Through interface repair post-treatment, the study demonstrates significant improvements in both the onset potential and fill factor (FF) of the PEC devices. Experimental results reveal that interface repair optimizes the crystallinity of the In_2S_3 layer, reduces interfacial defect states, and promotes efficient charge separation at the semiconductor/electrolyte interface. Electrochemical impedance spectroscopy (EIS) results show a notable reduction in charge transfer resistance and an increase in carrier lifetime after interface repair, while operando-dual working electrode (DWE) measurements confirm improved surface reaction kinetics and reduced recombination losses. This study provides new insights into the design of environmentally friendly buffer layers for PEC devices and offers a viable strategy for improving the efficiency of solar-driven energy conversion systems.

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Ultrafast-Sintered LLZO Membranes for high energy density ASSLBH. Zhang^{1,2}, F. Okur^{1,2*}, M. Klimpel^{1,2*}, K. V. Kravchyk^{1,2*}, M. V. Kovalenko^{1,2*}

¹Laboratory for Thin Films and Photovoltaics, Empa – Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland, ²Laboratory of Inorganic Chemistry, Department of Chemistry and Applied Biosciences, ETH Zürich, Vladimir-Prelog-Weg 1, CH-8093 Zürich, Switzerland

The field of all-solid-state lithium battery (ASSLB) research is rapidly shifting toward developing $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$ (LLZO)-based solid-state lithium metal batteries. To date, a new ultra-fast sintering (UF-sintering) method has been proposed recently to overcome the challenges associated with sintering LLZO SSEs. This study presents an in-depth analysis of the surface chemistry of UF-sintered LLZO using comprehensive techniques, including depth-profiling X-ray photoelectron spectroscopy (XPS) and focused-ion-beam time-of-flight secondary ion mass spectroscopy (FIB-TOF-SIMS). Our investigation uncovers a striking difference between the surface of UF-sintered and conventionally-sintered LLZO, revealing a predominant surface contamination by Li_2O up to *ca.* 40 nm depth in the case of UF processing. Comparative synchrotron X-ray diffraction data during UF and conventional sintering elucidate the origin of surface contamination. We propose a viable solution to this issue through an additional heat-treatment (HT) step at 900 °C after UF sintering, as corroborated by XPS, and FIB-TOF-SIMS measurements.¹

In this work, we demonstrate the methodology of the fabrication of self-standing, dense, 45 μm -thick LLZO membranes using UF-sintering technique. The membranes in Li/LLZO/Li symmetrical cell configuration exhibit a high critical current density of up to 12.5 mA cm^{-2} and maintain superior cycling stability for 250 cycles at a current density of 1 mA cm^{-2} , with an areal capacity limit of 1 mAh cm^{-2} . The electrochemical performance of LLZO membranes was also assessed in full cell configuration using a pyrochlore-type iron (III) hydroxy fluoride cathode.²

Figure 1. SEM images (A) before and (B) after UFS. (C) Calculated atomic ratio contributions based on depth-profiling XPS of UF-sintered LLZO membranes. (D) Corresponding O 1s areal fraction of LLZO, Li_2O , and C_{adv} of UF-sintered LLZO membranes without and with additional heat-treatment steps.

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Polar Polymers as Electrolytes in Lithium Metal Batteries

C. Zimmerli^{1,2}, F. Okur^{1,2*}, Y. Sheima^{1*}, K. Kravchyk^{1,2*}, D. Opris^{1,2*}, M. Kovalenko^{2,1*}

¹EMPA, ²ETH Zürich

Rechargeable lithium-ion batteries are used in most portable electronic devices and in electric vehicles, which are considered the future of transport. Conventional liquid electrolytes used in such batteries are associated with safety concerns due to their high volatility, flammability and toxicity. Solid-state polymer electrolytes (SSPE) can be considered a promising solution for the future generation of solid-state rechargeable batteries. Functionalized polysiloxanes allow the exploration of structure-property relationships, side group design, and thermal and dielectric properties, resulting in one of the highest permittivity for a polymer with a glass transition below room temperature^[1]. This work investigates the synthesis of Li-ion conductive polysiloxane-based polymers grafted with different polar groups and concentrations. This allowed us to identify several promising polymers, which, after the addition of lithium salt and crosslinking of the polymers, resulted in flexible, mechanically and electrochemically stable SSPE. The obtained modified polymers exhibit high ionic conductivities up to 0.375 mS cm⁻¹ at 60 °C and a Li-ion transfer number of 0.73, which is one of the highest reported for polymer electrolytes^[2].

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An Industrial Approach for the Synthesis of functionalized-Xylose via Direct Trans-acetalizationA. Bajramaj¹, M. Hedou^{1*}, R. Marti^{1*}¹HEIA-FR

The development of bio-based monomers is crucial for reducing the environmental impact of fossil-based plastics. However, existing methods¹, like dimethyldiglyoxylate xylose (DMGX) synthesis using aldehyde protection chemistry, often require harsh conditions and complex purification.

Here, we present a novel synthetic process for producing a xylose-derived monomer (acetal protection), diethyldiglyoxylate xylose (DEGX), via an trans acetalization reaction using ethyl diethoxyacetate (EDEA) as both a solvent and a reactant. This process was optimized using heterogeneous (Amberlyst-15) and lewis acid (FeCl₃) catalysis and achieve yields of up to 80%. The purification of DEGX was achieved through hydrolysis to diglyoxylic acid xylose (DGAX), followed by salt formation, yielding 50% of purified DGAX from xylose. Compared to the reference process based on glyoxylic acid and xylose (aldehyde protection), this approach avoids the use of non-recyclable aldehydes and hazardous acids, while enabling the recyclability of EDEA, which was recovered at 80% for reuse in subsequent batches. The final product shows high purity (92-97% determined by NMR), and its simplified purification steps improve industrial feasibility. Additionally, a preliminary exploration of flow chemistry was conducted, demonstrating its potential but highlighting challenges in ethanol removal and catalyst regeneration. This work establishes a scalable and sustainable alternative for bio-based monomer production.

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