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Phase Separation: A Versatile Tool for Designing Dynamic Polymer Networks

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Vitrimers are chemically crosslinked networks that can rearrange their topology without decreasing their crosslinking density thanks to exchangeable links present in the network. As a result, vitrimers can be reshaped and recycled at will, while displaying the superior properties of crosslinked polymers at service temperature. Very promising materials to create a circular economy of plastics and polymeric materials, vitrimers still display limitations that impact their transition towards industry, such as synthetic cost, high viscosity even at elevated temperatures, due to the Arrhenian temperature dependence of the melt viscosity, or moderate creep resistance at working temperatures in the case of low Tg materials.

Although many strategies have been reported to address these issues, it remains challenging to overcome a key tradeoff between improving the processability or the mechanical performance of vitrimers.

This lecture will present strategies that use phase separation to improve the processability and mechanical performance of dynamic polymer networks,[1-4] to upcycle polyolefin blends,[5] or to create self-healing, injectable hydrogels.[6]

[1] Röttger, M.; Domenech, T.; van der Weegen, R.; Breuillac, A.; Nicolaÿ, R.; Leibler, L., High-performance vitrimers from commodity thermoplastics through dioxaborolane metathesis. *Science* **2017,** *356*, 62-65.
[2] Formon, G. J. M.; Storch, S.; Delplanque, A. Y. G.; Bresson, B.; Van Zee, N. J.; Nicolay, R., Overcoming the Tradeoff Between Processability and Mechanical Performance of Elastomeric Vitrimers. *Adv. Funct. Mater.* **2023,** *33*, 2306065.
[3] Quinteros-Sedano, A.; Bresson, B.; Van Zee, N. J.; Nicolay, R., Improving the Thermomechanical Properties and Processability of Elastomeric Vitrimers Using Thermoreversible Organic Nanofillers. *ACS Mater. Lett.* **2024,** *6*, 877-884.
[4] Formon, G. J. M.; Jayaratnam, J.; Guibert, C.; Van Zee, N. J.; Nicolay, R., Cross-Linking Vitrimers after Melt Processing Using Supramolecularly Masked Dynamic Cross-Linkers. *Macromolecules* **2024,** *57*, 8277-8286.
[5] Vialon, T.; Sun, H.; Formon, G. J. M.; Galanopoulo, P.; Guibert, C.; Averseng, F.; Rager, M.-N.; Percot, A.; Guillaneuf, Y.; Van Zee, N. J.; Nicolay, R., Upcycling Polyolefin Blends into High-Performance Materials by Exploiting Azidotriazine Chemistry Using Reactive Extrusion. *J. Am. Chem. Soc.* **2024,** *146*, 2673-2684.
[6] Sun, H.; Gode, I.; Bonnard, M.; Liautard, V.; Pomes-Hadda, M.; Aime, S.; Chabaud, L.; Edera, P.; Guerinot, A.; Pucheault, M.; Nicolay, R., Self-Healing and Creep-Resistant Injectable Hydrogel from Aminoborinate Chemistry and Phase Separation. *ACS Mater. Lett.* **2025,** *7*, 2534-2540.

Optimizing Copolymer Microgels for Tunable Structural Color Formation

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Structural color formation in soft colloidal systems represents a promising approach toward stimuli-responsive photonic materials. In this study, we investigated the assembly of poly(N-isopropylacrylamide) (PNIPAm)-based microgels incorporating varying percentages of anionic (methacrylic acid), neutral (acrylamide), and cationic (2-(dimethylamino)ethyl methacrylate) comonomers to create multifunctional colloidal building blocks capable of forming dynamic structural colors. Through synthesis optimization and surfactant-mediated size control, we obtained libraries of copolymer microgels with precisely tailored particle diameter, surface charge, and stimuli-responsive swelling behavior.

We generated structural colors across the visible spectrum by colloidal crystal assembly through thermal annealing and modulated the interparticle spacing and consequently the reflected wavelengths by changing the microgel concentration. Additionally, by fine-tuning the microgel responsiveness, we engineered materials with precise wavelength shifts in the reflected color upon environmental stimuli (temperature or pH).

Our findings provide key insights into the interplay between microgel responsiveness, compressibility, and the resulting structural color formation that are expected to support advanced multifunctional colloidal sensors, coatings, and optical tags.

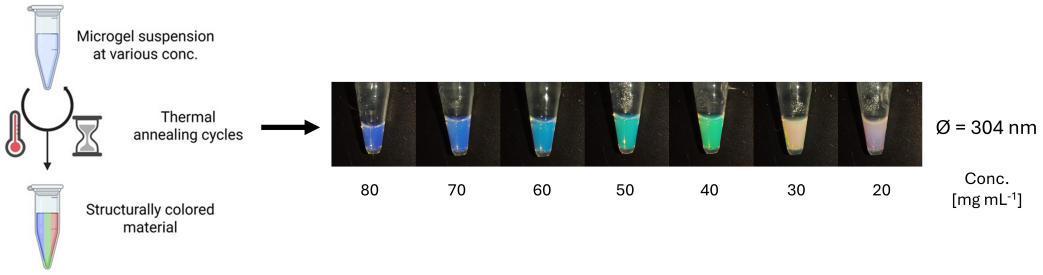


Figure 1: Schematic representation of structural color formation through thermally induced assembly of copolymer microgels. The reflected wavelengths are dependent on the microgel size and concentration.

[1] M. Kraus, M. Malekovic, I.A. Dinu, C.G. Palivan, *Small Science*, **2026**, 6

[2] M. Hildebrandt, D.P. Thuy, J. Kippenberger, T.L. Wigger, J.E. Houston, A. Scotti, M. Karg, *Soft Matter*, **2023**, 19

[3] Y. Xia, S. Gao, H. He, X. Wang, Z. Zeng, B. Chen, N. Zhou, M. Cao, S. Wang, *Journal of Physical Chemistry*, **2020**, 124

Toward Chemical Processors: Programmable Reaction-Diffusion Networks in Silicon Microreactors

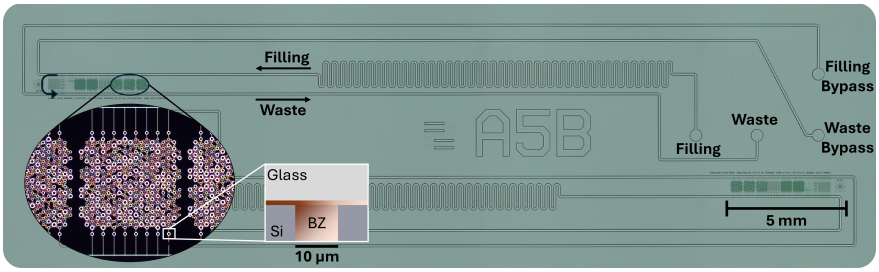
S. Agostini[1,2], V. Zarth[1], M. Fasching[1], P. Schwaller[2,3], J. Pérez-Mercader[4], A. W. Knoll[1]*, H. Wolf[1]*

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Chemical systems capable of autonomous spatiotemporal dynamics offer an energy efficient physical substrate for information processing beyond conventional electronic materials. Here, we present a microfabricated silicon platform that confines the oscillatory Belousov–Zhabotinsky reaction in networks of coupled microreactors, forming an excitable reaction–diffusion medium for chemical signal processing.

Within the silicon microreactor platform, micrometer-scale reactors connected by nanochannels support propagating chemical excitation waves that serve as signals. We experimentally demonstrate wave transmission between coupled reactors, geometry-defined propagation pathways, delayed signal arrival, signal regeneration, and fan-out in branching network structures. These functions arise from the nonlinear autocatalytic dynamics of the Belousov–Zhabotinsky reaction, which provide intrinsic thresholding and amplification, while the microfabricated network geometry defines connectivity and coupling strength.

Using the same silicon microreactor platform, we realize a chemical XOR operation based on coincident excitation, demonstrating nonlinear signal integration in a spatially extended chemical medium. This result shows that engineered reaction–diffusion networks can implement elementary logic-like functionality through collective chemical dynamics.



To explore a route toward dynamic programmability, we perform complementary macroscopic experiments showing that electrochemical biasing can modulate Belousov–Zhabotinsky oscillations through locally generated activator molecules that are amplified by the reaction network [1]. This electrochemical control is not yet integrated into the silicon microreactor platform, but it motivates future architectures in which fixed microreactor geometry defines the computational graph and patterned electrodes provide addressable, programmable control.

Together, these results establish silicon-based chemical microreactor networks as active materials for reaction–diffusion signal processing. They represent a step toward chemically active processor architectures capable of nonlinear signal propagation, integration, and adaptive response, with potential applications in sensing, autonomous operation, and unconventional information processing.

[1] S. Agostini, P. Schwaller, J. Pérez-Mercader, A. Knoll, H. Wolf. From Microcurrents to Macrodynamics: Harnessing Mixed Potentials for Large, Tunable Acceleration of Belousov–Zhabotinsky Oscillations. ChemRxiv. 05 March 2026. DOI: https://doi.org/10.26434/chemrxiv-2025-wrt8d/v4

Unlocking Aromatic Monomers by Living Cascade Ring-Opening Polymerization

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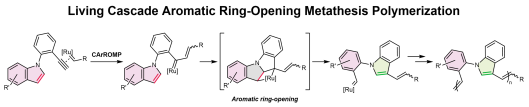
Aromatic molecules are among the most ubiquitous and structurally robust motifs in chemistry, yet their direct implementation as monomers in metathesis polymerization has long been considered unattainable due to their substantial aromatic stabilization. Overcoming this intrinsic stability without complete loss of aromaticity represents a longstanding challenge in polymer synthesis.

Here, we report the ring-opening metathesis polymerization of aromatic monomers enabled by a cascade process. The monomers are built on an indole scaffold bearing a phenyl acetylene handle that functions as a kinetic trigger. Rapid alkyne insertion initiates a selective intramolecular cascade that redistributes energy and enables aromatic ring opening with regeneration of an aromatic motif. Rather than directly disrupting aromatic stabilization, this strategy reorganizes it to enable incorporation into the polymer backbone.

Using commercially available Grubbs third-generation catalyst (G3), we achieve controlled metathesis polymerization of these aromatic monomers with high cascade efficiency. Monomers bearing both electron-donating and electron-withdrawing substituents undergo successful polymerization, demonstrating broad functional group tolerance. By systematically varying substituents on the monomer framework, we further modulate the polymerization rate by up to 15-fold, demonstrating precise kinetic control over the cascade process. Block copolymer synthesis further supports the living character of this cascade aromatic ring-opening metathesis polymerization.

Mechanistic studies based on in situ NMR monitoring and DFT calculations reveal that alkyne insertion, rather than aromatic ring opening, constitutes the rate-determining step. Intramolecular indole coordination slightly reduces aromaticity, lowering the barrier for ring opening and facilitating the cascade process under metathesis conditions. These findings demonstrate that aromatic ring opening is accessed through kinetic regulation rather than direct disruption of aromatic stabilization.

Collectively, this work establishes a general strategy for achieving aromatic ring opening in the metathesis polymerization of aromatic monomers, transforming aromatic stability from a synthetic constraint into a design element.



[1] R. Guo; J. E. McGrath. 5.17 - Aromatic Polyethers, Polyetherketones, Polysulfides, and Polysulfones. In Polymer Science: A Comprehensive Reference, Matyjaszewski, K., Möller, M. Eds.; Elsevier, 2012; pp 377-430.

[2] T. Yokozawa; Y. Ohta. Chem. Commun. 2013, 49 (75), 8281-8310.

[3] Y.-L. Su; L. Yue; H. Tran; M. Xu; A. Engler; R. Ramprasad; H. J. Qi; W. R. Gutekunst. J. Am. Chem. Soc. 2023, 145 (25), 13950-13956.

[4] P. D. Zeits; T. Fiedler; J. A. Gladysz. Chem. Commun. 2012, 48 (64), 7925-7927.

[5] M. K. Cyrański. Chem. Rev. 2005, 105 (10), 3773-3811.

Molecular Dynamics Simulation of the Passivation Process of Hydroxylated Tin Oxide for Solar Cell Devices

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Tin oxide (SnO2) semiconductor is frequently used in solar cell devices as an electron transport layer (ETL). However, due to its inherent highly reactive nature, interface passivation is required to ensure stability and prevent undesirable reactions with the active layer. In this context, the use of self-assembled monolayers (SAMs) with organic additives has been explored to protect the surface of the ETL.[1]

Notwithstanding, the molecular arrangement of these SAMs, as well as the reactive processes at the surface of SnO2, presents a high-dimensional problem that requires electronic structure methods with high accuracy and remains a challenge in the scientific community.[2]

In this work, we constructed a machine learning force field (MLFF) based on first-principle method to understand the reactive mechanisms involved in the hydroxylation process of SnO2 as well as the interactions between hydroxylated SnO2 and typical additives utilized in SAMs for surface passivation.

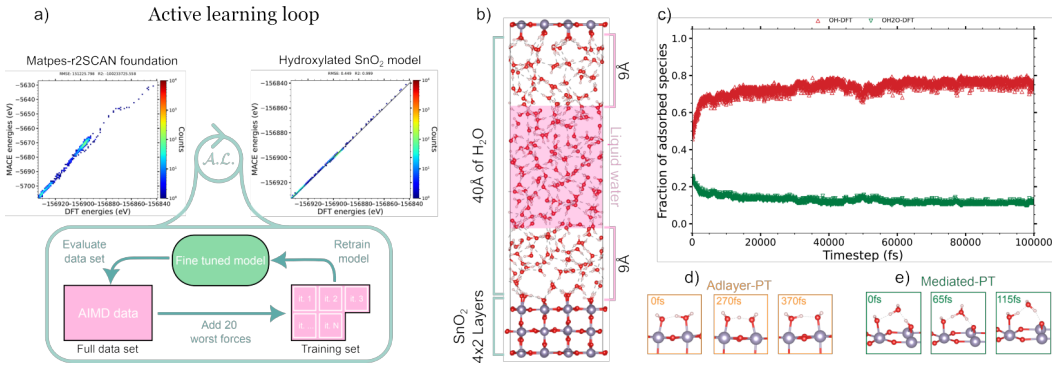


Figure 1: a) Representation of the active learning loop, b) representation of the simulated system, c) variation of hydroxylation of the surface (red) et adsorbed water (green) in function of simulation time, d) and e) mechanisms of surface proton exchange.

References:

[1] Park, S.M., Wei, M., Lempesis, N. et al. Nature, 624, (2023) 289–294

[2] M. Jia, Y.B. Zhuang, F. Wang, C. Zhang, J. Cheng, Precis. Chem., 2, 12, (2024) 644–654

Project HEOCat: Engineering Porous High-Entropy Oxides for Sustainable Energy and Environmental Applications

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Multi-cationic oxides containing five or more elements have recently attracted significant attention as the field of high-entropy materials (HEMs) expands beyond its original focus on high-entropy alloys (HEAs) to encompass oxide systems. High-entropy oxides (HEOs) offer a unique combination of compositional complexity, tunable electronic structures, and enhanced thermal and chemical stability, making them promising materials for a wide range of energy and environmental applications. Despite their considerable potential, HEOs have seen only limited exploration in heterogeneous catalysis and adsorption technologies. A major bottleneck is the absence of robust and scalable synthesis methods that can reliably produce porous, high-surface-area HEOs tailored for these applications.

Through support from the Swiss National Science Foundation (SNF) Ambizione program, this project addresses these challenges by developing versatile synthesis strategies for porous high-entropy oxides. Particular emphasis are on approaches that can produce HEOs with the high surface areas and accessible active sites required for catalytic and adsorption applications.

Given the vast compositional and synthetic parameter space associated with HEOs, conventional trial-and-error optimization approaches are inefficient. Therefore, the project utilizes high-throughput synthesis and characterization capabilities available in Switzerland, like SwissCAT+, to accelerate materials discovery and optimization.

Building upon these synthetic advances, the project investigates how high-entropy oxides can be tailored for two key application areas. First, we explore their use in heterogeneous catalysis, where their compositional complexity may generate unique active sites, enhance catalyst stability, and improve resistance to sintering and deactivation, specifically CO2 hydrogenation as a model reaction. Second, we will examine their potential as adsorbent materials separation processes, where tunable surface chemistry and defect structures may enable improved adsorption capacity and selectivity. Here, in situ characterization techniques such as XRD and XAS are utilized to understand how these materials uniquely behave under operating conditions.

Through these studies, the project seeks to establish fundamental design principles for high-entropy oxides and expand their application in sustainable catalytic and separation technologies.

[1] C. M. Rost, E. Sachet, T. Borman, A. Moballegh, E. C. Dickey, D. Hou, J. L. Jones, S. Curtarolo and J.-P. Maria, *Nat. Commun.*, 2015, **6**, 8485.

[2] Y. Pan, J.-X. Liu, T.-Z. Tu, W. Wang and G.-J. Zhang, *Chem. Eng. J.*, 2023, **451**, 138659.

[3] A. J. Knorpp, A. Zawisza, S. Huangfu, A. Borzì, A. H. Clark, D. Kata, T. Graule and M. Stuer, *RSC Adv.*, 2022, **12**, 26362–26371.

[4] A. J. Knorpp, P. Allegri, S. Huangfu, A. Vogel and M. Stuer, *Inorg. Chem.*, 2023, **62**, 4999–5007.

[5] A. J. Knorpp, M. Mielniczuk, M. Nikolic, A. Vogel, R. Figi, C. Schreiner, A. Borgschulte and M. Stuer, *Eur. J. Inorg. Chem.*, 2024, **27**, e202400476.

Accelerated Transformation in Chemistry and Energy

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Process improvement, mobility, sustainability, and electricity as well as chemicals generation (P-to-X) are pivotal fields of interest in transforming chemistry and energy. Development of lighter batteries with increased energy density, more efficient photovoltaics, porous storage materials, fuel cell catalysts and membranes, optoelectronic nanomaterials, semiconductor materials, porous separation materials, and CO_2 hydrogenation catalysts has become pivotal research topics over the past years and are enabled by Chemspeed's high-throughput and high-output automated, digitalized solutions.

This presentation covers a selection of case studies such as battery inks, perovskites, quantum dots, thermoelectric materials, porous materials, catalysts in conjunction with showcasing agentic automated workflows (Fig. 1) and end-to-end connected laboratories for Design-Make-Analyze-Test-Learn (DMATL).

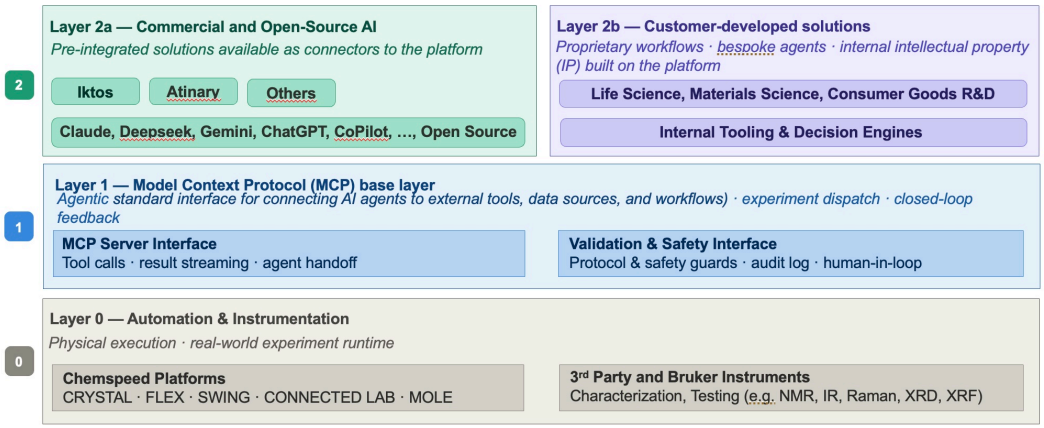


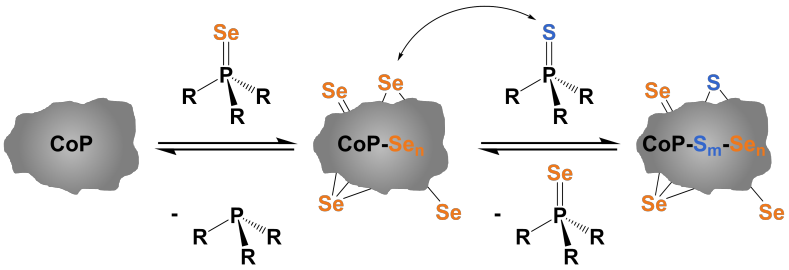
Fig. 1 - Artificial Intelligence (AI) Agents and Model Context Protocol (MCP) Servers – A Plug & Play Strategy to increase domain knowledge and to enable your existing AI infrastructure to directly control and monitor laboratory workflows.

Controlled Dual Doping of Transition Metal Phosphide Surfaces

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Today`s industrial production of chemicals is still heavily reliant on noble metal catalysts. In search of more sustainable alternatives, recent research suggests that transition metal phosphides (TMPs) can efficiently catalyze reactions such as hydrogenations or water splitting.[1-2] However, catalytic activity and stability still need to be further improved. This may be possible by doping TMPs with heteroatoms.[3-4] In particular, doping with multiple elements can provide synergistic effects in catalysis.[5-6] To implement such doping strategies effectively for TMP catalysis, more insight into the nature of different doping sites and what controls doping of these sites is needed. However, this knowledge is challenging to obtain with current doping methods that offer little control over the doping process. Herein, we show that our recently reported method for sulfur-doping of cobalt phosphide (CoP)[7] can be further developed to allow dual-doping of a CoP surface with multiple different chalcogenide heteroatoms. Our approach allowed us to gain more insight into the nature of the different doping-sites available on amorphous CoP material. Furthermore, our results provide a better understanding of the factors that govern the dual-doping outcome. Our work therefore shows the road for a more systematic development of new multi-doped TMP catalysts.



[1] S. T. Oyama, T. Gott, H. Zhao, Y.-K. Lee, *Catalysis Today,* **2009**, 143, 94-107.
[2] Y. Shi, B. Zhang, *Chem. Soc. Rev.*, **2016**, 45, 1529-1541.
[3] S. M. El-Refaei, P. A. Russo, N. Pinna, *ACS Appl. Mater. Interfaces,* **2021**, 13, 22077-22097.
[4] Y. Sun, T. Zhang, C. Li, K. Xu, Y. Li, *J. Mater. Chem. A,* **2020**, 8, 13415-13436.
[5] H. Bai, D. Chen, Q. Ma, R. Qin, H. Xu, Y. Zhao, J. Chen, S. Mu, *Electrochem. Energy Rev.,* **2022**, 5:24
[6] Y. Lin, Y. Pan, J. Zhang, Y. Chen, K. Sun, Y. Liu, C. Liu, *Electrochim. Acta*, **2016**, 222, 246-256
[7] N. A. Arnosti, V. Wyss, M. F. Delley, *J. Am. Chem. Soc.*, **2023**, 145, 23556-23567.

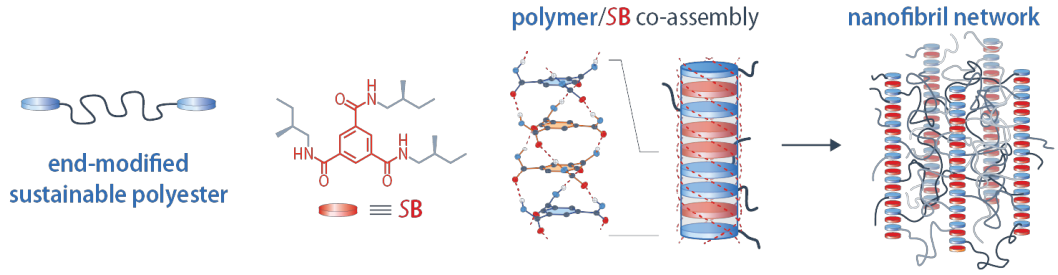
Chirality-Controlled Supramolecular Modification of High-Molar-Mass Polyester for Improved Processing and Performance

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The plastic waste crisis is one of the biggest challenges for mankind. As chemically recyclable and biodegradable materials that can be produced from renewable resources, aliphatic polyesters are considered promising sustainable alternatives for conventional plastics. However, their mass application is impeded by their inferior processability and mechanical properties. Supramolecular polymer modification can provide solutions in this regard, if its limitation to low-molar-mass polymers is overcome and dynamic exchange of supramolecular ligands is tailored appropriately.

We investigated materials based on a sustainable polyester modified with benzene-1,3,5-tricarboxammide (BTA) end groups and blended with a low-molar-mass BTA additive, which we have shown to be a versatile strategy to overcome the molar-mass limitations of supramolecular polymers.[1,2] Due to the helical arrangement of the amide hydrogen bonds around the central benzene stack as a source of frustration, BTA co-assembly results in defined one-dimensional supramolecular columnar aggregates via ditopic multivalent hydrogen bonding. The supramolecular polymer network reinforced with these BTA nanofibrils shows a rubbery behavior at temperatures significantly above the polymer melting point as well as improved melt strength, which is relevant to broaden the processing possibilities. During melt deformation, however, the exchange dynamics of BTA molecules in the columnar stacks is an important feature. Using the chiral BTA derivative *N*,*N*',*N*''-tris((*S*)2-methylbutyl)benzene-1,3,5-tricarboxamide (*S*B), we can tailor the exchange dynamics to be fast enough to allow for a reorganization of the supramolecular aggregates but slow enough to prevent materials flow. This leads to melt-processing opportunities that are not possible for the pristine polymer. Our results show the importance of supramolecular motif design for properties and performance of the final material.



[1] Daniel Görl; Shuichi Haraguchi; Yevhen Hryshunin; Sophia Thiele; Giorgia Scetta; Alexandre Simula; Matthieu Wendling; Oguzhan Oguz; Nicolas Candau; Torne Tänzer; Marianne Liebi; Christopher J. G. Plummer; Holger Frauenrath, *Nature Communications*, **2025**,16, 217-230.

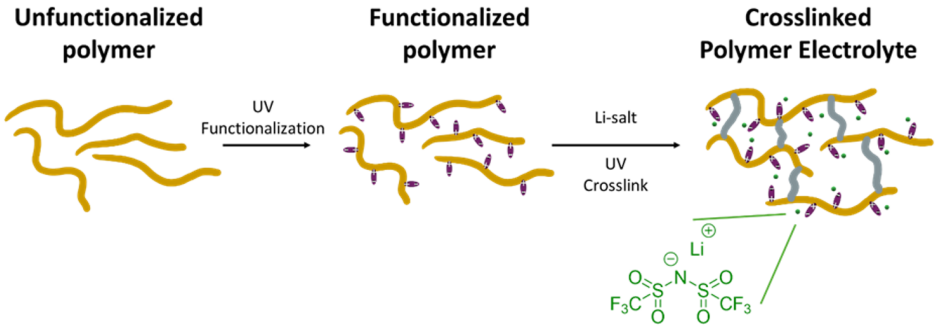
[2] Sophia Thiele; Michael Giffin; Matthieu Wendling; Daniel Görl; Christopher J. G. Plummer; Holger Frauenrath, *Organic Chemistry Frontiers*, **2025**, 12, 5395-5413.

Polar Polymers as Electrolytes in Lithium Metal Batteries

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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 pose safety concerns due to their high volatility, flammability, and toxicity. Solid-state polymer electrolytes (SSPE) can be considered a cheap, scalable and safe 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 and characterization of Li-ion conductive polysiloxane-based polymers grafted with different polar groups and concentrations in battery electrolytes (Figure 1). This allowed us to identify several promising polymers that, upon addition of a lithium salt and crosslinking, yielded flexible, mechanically and electrochemically stable SSPE. The obtained modified polymers exhibit ionic conductivities up to 0.375 mS cm^{-1} at 60 °C, Li-ion transference number of 0.73, which is one of the highest reported for polymer electrolytes, electrochemical stability up to 5 V towards Lithium metal and stable charge/discharge cycles of symmetric cells over 1500 h. [2] The main advantage is the replacement of PVDF in cathode materials with our modified poylmers to obtain fluorine-free binder material with excellend adhesion to the electrolyte.



[1] Y. Sheima, Y. Yuts, H. Frauenrath, D.M. Opris, Macromolecules, **2021**, 54, 5737–5749.

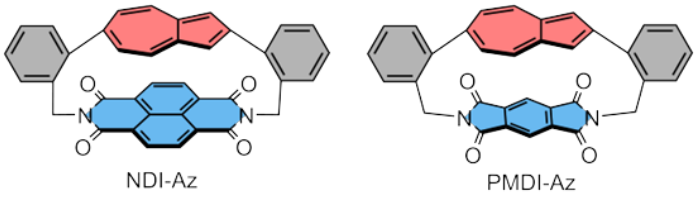
[2] F. Okur, Y. Sheima, C. Zimmerli, H. Zhang, P. Helbling, A. Fäh, I. Mihail, J. Tschudin, D. M. Opris, M. Kovalenko, K. Kravchyk, ChemSusChem, **2024**, 17.

Exploration of Asymmetric Paracyclophanes Functionalized with Azulene and NDI or PMDI

G. Graf[1], M. Mukherjee[2], E. Zyaee[3], C. Negrete-Vergara[1], V. Slama[2], H. Frey[3], T. Feurer[3], U. Röthlisberger[2]*, S. Liu[1]*

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Molecular devices such as diodes typically consist of an electron donor (D) and acceptor (A) linked by a bridge. The bridge acts as a separator, ensuring a physical distance between the donor and acceptor units, so that current can only flow in one direction. Upon photoexcitation, an intramolecular charge-transfer (CT) occurs. A good understanding of these CT processes is crucial for developing new molecular devices.[1] Paracyclophanes have emerged as attractive scaffolds for molecular devices because their rigid and tunable architectures are well-suited for probing CT interactions.[2] In this work, we designed two novel paracyclophanes that contain two parallel π-systems, forming a D-A ensemble (see figure below). The electron donor is composed of azulene (Az), a blue emitter with a large inherent dipole moment.[3] On the other hand, naphthalene-tetracarboxylic diimide (NDI) and pyromellitic diimide (PMDI) have both a high electron affinity and can serve as efficient electron acceptors. When combined, they can undergo photoinduced through-space charge transfer (TSCT), resulting in a substantial increase in electric dipole moment. A detailed study of single-crystal structures and redox and optical properties, supported by DFT calculations, showed that the TSCT interactions are strongly affected by the geometry and spatial alignment of D and A units within the paracyclophane framework.



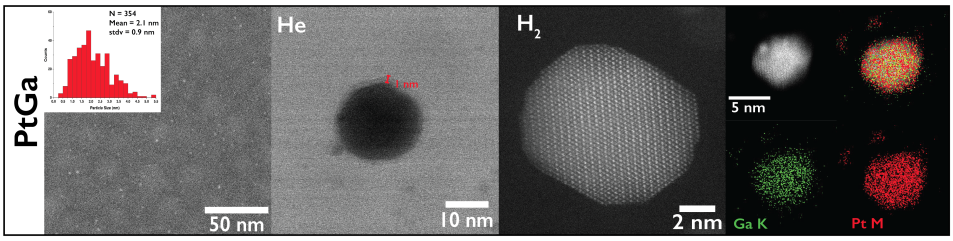
[1] Sascha Ullbrich, Johannes Benduhn, Xiangkun Jia, Vasileios C. Nikolis, Kristofer Tvingstedt, Fortunato Piersimoni, Steffen Roland, Yuan Liu, Jinhan Wu, Axel Fischer, Dieter Neher, Sebastian Reineke, Donato Spoltore, Koen Vandewal, *Nature Materials*, **2019**, 18, 459–464. [2] Z. Wang, Y. Liu, X. Quan, W. Zhang, R. Tan, H. Gu, C. Sheng, C. Duan, P. Xing, J. H. Wan. *Angewandte Chemie – International Edition*, **2025**, 64, e202413295. [3] Hanshen Xin, Bin Hou, Xike Gao, *Accounts of Chemical Research*, **2021**, 54, 1737–1753.

Surface Organometallic Chemistry on a MEMS Chip: Operando TEM Study of Dynamics of Alloyed PtGa Nanoparticles during Propane Dehydrogenation

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Establishing structure-activity relationships in heterogeneous catalysis remains challenging due to multi-component complexity.[1] Surface Organometallic Chemistry (SOMC) minimizes this complexity, enabling the formation of well-defined (bi)metallic nanoparticles with tailored interfaces.[2] However, *operando* (Scanning) Transmission Electron Microscopy ((S)TEM) imaging of heterogeneous catalysts is often hindered by standard sample preparation (sonication/drop-casting). These conventional methods cause inhomogeneous catalyst distribution and charging effects from poor physical contact between the catalyst and the chip, compromising spatial resolution.[3]To overcome these limitations, the SOMC approach is used to synthesize tailored (bi)metallic catalysts directly onto an Al_2O_3-coated MEMS chip,[4] facilitating a uniform dispersion of nanoparticles, and therefore a more reproducible correlation of structure-activity relationships.



We applied this novel methodology to study alloyed PtGa NPs supported on a Al_2O_3-coated MEMS chip for propane dehydrogenation.[5] Using a double aberration Cs-corrected (S)TEM operated at 300 kV and equipped with a dual SDD-EDX detector system, we monitored the structural dynamics of alloyed PtGa nanoparticles in different gas atmospheres. under He, High-angle annular dark-field STEM imaging revealed that air-exposed particles exhibit a core-shell like structure with an amorphous GaO_x shell, which is then reduced when exposed to H_2 at 600°C. The successful formation of a homogenoeus alloy is confirmed by STEM EDX elemental mapping (Figure 1). When exposed to the diluted propane mixture, a dynamic behaviour assigned to the presence of Ga alloyed species (from DFT-based metadynamics calculation) and the concomitant formation of a metastable Pt_2C-phase are observed. Additionally, the presence of "holes" or missing atoms is observed, likely due to the formation of stiff carbon-chains limiting the movement of the Ga atoms.

[1] Schlögl R., *et al.*; *Angewandte Chemie International Edition,* **2015**, 54, 3465-3520.
[2] Copéret C., *et al.*; *Accounts of Chemical Research*, **2019**, 52, 1697-1708.
[3] Yue S., *et al.*; *Nature Communications*, **2024**, 15, 4678.
[4] Brack E., *et al.; Journal of the American Chemical Society*, **2026**, 148, 19, 19722-19729.
[5] Sakamoto K., *et al.*; *Journal of the American Chemical Society*, **2025**, 147, 25, 22041-22052.

Multimetallic High-Entropy Spinel Oxides as Tunable Catalysts for CO_2 Hydrogenation

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High-entropy oxides (HEOs) are a novel type of high-entropy materials that consist of five or more cations in near equimolar ratios and distributed within a single crystalline lattice [1]. Their unique combination of structural stability, lattice distortion, tunable redox behavior, and synergistic multication effects make them as promising alternatives for applications in energy conversion and catalysis [2,3]. However, due to the large compositional space, their rational design and scalable synthesis still remain challenging. In this work, porous HEOs are tailored for thermocatalytic CO_2 hydrogenation into value-added products, such as methane, methanol, carbon monoxide and hydrocarbons. High-entropy layered double-hydroxides (HE-LDHs) were synthesized by hydrothermal/co-precipitation methods as catalysts precursors and then calcined to obtain the corresponding spinel oxides [4]. X-ray diffraction and scanning electron microscopy (SEM/EDX) were used to identify the structure, morphology and homogeneous distribution of cations in HEO samples, while N_2 physisorption confirmed their large surface area by BET analysis. Catalytic testing was performed in a fixed-bed reactor under CO_2 hydrogenation conditions for selected HEO compositions and molar ratios, comprising of at least 5-10 cations of non-noble metals: Al, Mg, Cr, Fe, Co, Ni, Cu, Zn. Local coordination and oxidation states during H_2 activation and reaction conditions were assessed by *operando* X-ray absorption spectroscopy (XAS), revealing the formation of small multimetallic domains exsolved from the high-entropy matrix which act as the main active sites. Overall, these findings highlight the potential of high-entropy oxides as tunable platforms for CO_2 hydrogenation, with comparable performance to state-of-the-art catalysts, and provide a basis for more rational compositional designs through advanced characterization techniques.

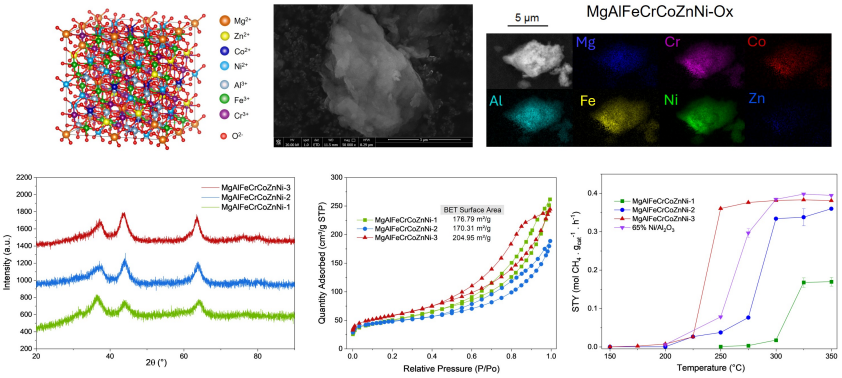


Figure 1. Characterization (SEM/EDX, XRD, BET analysis) of MgAlFeCrCoZnNi high-entropy spinel oxides and their catalytic performance for CO_2 methanation

[1] C. M. Rost, E. Sachet, T. Borman, A. Moballegh, E. C. Dickey, D. Hou, J. L. Jones, S. Curtarolo, J.-P. Maria, *Nature Communications*, **2015**, 6, 8485. [2] Y. Pan, J.-X. Liu, T.-Z. Tu, W. Wang, G.-J. Zhang, *Chemical Engineering Journal*, **2023**, 451, 138659. [3] Y. Wang, J. Mi, Z.-S. Wu, *Chem Catalysis,* **2022**, 2, 1624-1656. [4] A. J. Knorpp, M. Mielniczuk, M. Nikolic, A. Vogel, R. Figi, C. Schreiner, A. Borgschulte, M. Stuer, *European Journal of Inorganic Chemistry*, **2024**, 27, e202400476.

Linking Thermal Aging–Induced Structural Changes to Ammonia Speciation in VO_x–WO_x/TiO_2 Catalysts

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The combination of vanadium oxides (VO_x) with titania (TiO_2) constitutes a benchmark class of heterogeneous catalysts for industrially relevant reactions, including the selective catalytic reduction of NO_x with NH_3 (NH_3-SCR) and hydrocarbon oxidation reactions. Its performance originates from synergistic interactions between the redox properties of dispersed VO_x species and the acidic properties of the material[1]. While titania inherently provides Lewis acidity, the incorporation of VO_x and promoter tungsta generates both new Lewis-bound ammonia (LNH_3) as well as Brønsted–bound ammonium species (BNH_4^+)[2]. Thermal aging has been shown to induce catalyst activation, but further structural transformations ultimately lead to catalyst deactivation[3]. However, the dynamic nature of VO_x–TiO_2 surfaces has obscured a detailed molecular-level understanding of these processes. Here, we address this gap by elucidating the influence of thermal aging on active-site speciation and distribution, specifically with operando spectroscopic methods combined with the modulated excitation approach (ME)[2,4].

Catalysts were prepared by wet impregnation using aqueous solutions of ammonium metavanadate and metatungstate corresponding to 2 wt% V_2O_5 and 10 wt% WO_3, respectively, onto commercial DT52 and DT51 titania supports. After drying, the resulting powders were calcined at 450 °C, and aliquots were aged in air for 16 h at different temperatures. The catalytic performance for NH_3-SCR was evaluated in a fixed-bed powder reactor over the temperature range of 100–550 °C.

We investigated the surface chemistry of this catalytic system using diffuse reflectance infrared spectroscopy (DRIFTS) under NH_3-SCR conditions, combined with a modulated excitation (ME) approach to distinguish active from spectator species. The LNH_3/BNH_4^+ ratio obtained from DRIFTS increases with aging temperature, passing through a maximum at 550 °C. At higher temperatures, anatase-to-rutile transformation reduces the available surface area, leading to diminished catalytic performance above 650 °C. In addition to this phase transition, XRD reveals the crystallization of tungsta, indicating temperature-induced mobility of V and W species, while Raman spectroscopy evidences V and W rearrangement already at lower temperatures, which results in the alteration of surface acid sites. This systematic evolution upon aging, combined with advanced operando spectroscopy, enables correlation of specific structural motifs with catalytic activity and selectivity.

[1] J.-K. Lai, I. E. Wachs, ACS Catalysis, 2018, 8, 6537–6551.
[2] A. Marberger, D. Ferri, M. Elsener, O. Kröcher, Angewandte Chemie International Edition, 2016, 55, 11989–11994.
[3] A. Marberger, M. Elsener, R. J. G. Nuguid, D. Ferri, O. Kröcher, Applied Catalysis A: General, 2019, 573, 64–72.
[4] A. Urakawa, T. Bürgi, A. Baiker, Chemical Engineering Science. 2008, 63, 4902–4909.

Energy Transfer in Lanthanide-doped core/shell/shell Zirconia Nanocrystals

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Zirconia (ZrO_2) nanoparticles are emerging as a robust host material for optical applications due to their high thermal and chemical stability and large band gap. (1) While lanthanide doping has been widely explored in fluoride hosts such as $NaYF_4$ and $NaGdF_4$, these materials leach fluoride and lanthanide ions in aqueous environments. In contrast, zirconia offers a more stable and biocompatible matrix for biomedical applications.

This work focuses on co-doping zirconia nanocrystals with Europium(III) and Terbium(III) ions, with control over dopant location in core/shell/shell structures. The introduction of a zirconia shell significantly enhances the emission properties of the lanthanide dopants. (2) We present here the synthetic advances that allow access to core/shell and core/shell/shell structures and investigate the energy-transfer process between Eu^{3+} and Tb^{3+}. These engineered structures minimise quenching from surface-related defects and improve energy-transfer efficiency. Additionally, we demonstrate that emission colour tuning can be achieved by varying the excitation wavelength (fig.(b) and (c)), further expanding the functional versatility of these materials. These results provide insight into dopant placement strategies for advanced photonic and biomedical applications.

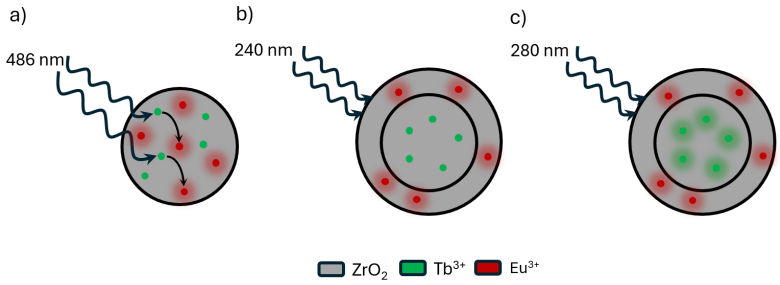


Figure 1: (a) Schematic representation of co-doped zirconia nanoparticles under irradiation at 486 nm showing energy transfer process between Tb^{3+} to Eu^{3+}, (b) and (c) colour tuning achieved by changing the excitation wavelength between 240 nm and 280 nm.

[1] C. Seno, N. Reichholf, J. De Roo, Journal of the American Chemical Society, 2024, 146(30), 20550-5.

[2] N. Reichholf, S. Horta, J. De Roo, ACS nano, 2025, 19(33), 30371-82.

Development of Microgram-Scale ^{226}Ra Targets for Precision Muonic Atom Spectroscopy

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The absolute nuclear charge radius of ^{226}Ra is a critical parameter required to interpret atomic parity violation experiments.[1,2] Muonic atom spectroscopy provides a sensitive method for extracting absolute nuclear charge radii. Because the Bohr radius is ~207 times smaller for muonic atoms, they exhibit an enhanced sensitivity to nuclear finite size effects by a factor of ~10^7. However, integrating this technique with a highly radioactive isotope like ^{226}Ra introduces strict radiological safety constraints, limiting the permissible target mass to the μg scale.

To overcome this limitation, spectroscopic measurements at the μg scale are achieved by exploiting muon transfer reactions and the Ramsauer–Townsend effect within high-pressure H_2-D_2 mixtures.[3,4] As a consequence of this mass limit, the target material must be prepared as an ultra-thin layer without surface contaminants, ensuring that diffusing muonic atoms can reach the radium nuclei without prior interception. Furthermore, deposition onto a low-Z backing suppresses background emissions that would otherwise obscure the ^{226}Ra signal. While minimizing deposition time and maintaining high yields is essential to prevent the radiolytic effects observed in the previous study of molecularly plated 5 μg ^{226}Ra targets prepared by molecular plating,[5] executing these iterative optimizations is restricted by the isotope's high radioactivity. Consequently, this work employs natural Ba as a non-radioactive chemical homologue to safely map the deposition parameters.

In this study, we present a framework for the fabrication and characterization of ultra-thin, μg scale targets on low-Z carbon-based backings, establishing the experimental conditions required to control and minimize radiolysis.

[1] M. Nuñez Portela *et al.*, *Hyperfine Interact.*, **2013**, 214, 157–162.

[2] M. Fan, C. A. Holliman, A. L. Wang, A. M. Jayich, *Phys. Rev. Lett.*, **2019**, 122, 223001.

[3] F. Mulhauser *et al.*, *Phys. Rev. A*, **2006**, 73, 034501.

[4] L. Antwis *et al.*, *Sci. Rep.*, **2025**, 15, 6939.

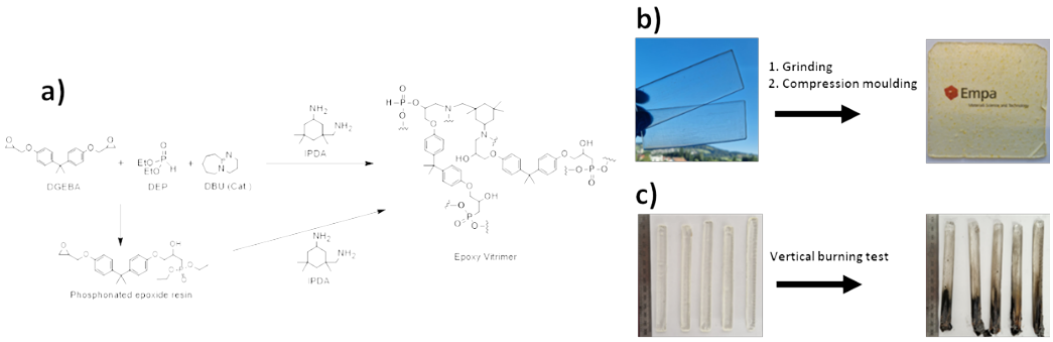
[5] E. A. Maugeri, N. Cerboni, A. Knecht, *EPJ Web Conf.*, **2025**, 327, 01005, 2025.

Transphosphonate Exchange-Enabled Recyclable Flame-Retardant Epoxy Thermosets

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Transphosphonate-based covalent adaptable networks (CANs) represent an emerging class of polymers that combine reprocessability, thermal stability, and intrinsic flame retardancy while maintaining the mechanical performance of conventional thermosets[1]; however, the chemical interactions inside the matrix governing network rearrangement and flow behavior remain insufficiently understood[2], limiting their broader application. This work is aimed at obtaining a reprocessable epoxy resin exhibiting intrinsic flame retardancy leveraging the transphosphonate exchange dynamic chemistry. Detailed structural characterization of the networks reveals their ageing characteristics and impact on long term thermomechanical performance. An efficient synthesis route based on commercially available precursors is employed and the phosphorus content is adjusted to ensure both efficient reprocessability and flame retardancy. The reprocessability is demonstrated through compression moulding and the fire safety through UL94 vertical burning test achieving a V0 classification at 6wt% of phosphorus. Spectroscopical techniques reveal changes in chemical environment and the kinetics of network topology rearrangement.



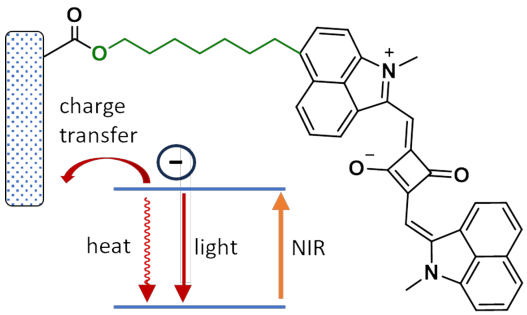
[1] W. W. Klingler, V. Rougier, Z. Y. Huang, D. Parida, S. Lehner, A. Casutt, D. Rentsch, K. B. Hedlund, G. A. Barandun, V. Michaud, S. Gaan, Chemical Engineering Journal, 2023, 466, 143051.
[2] Y. Spiesschaert, C. Taplan, L. Stricker, M. Guerre, J. M. Winne, F. E. Du Prez, Polymer Chemistry, 2020, 11, 5377–5385.

Hydroxy-Functionalized Near-Infrared Squaraine Dyes for Advanced Organic Conjugates and Hybrid Materials

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Far near-infrared squaraine dyes absorbing beyond 900 nm offer promising purpose of use in sensing and imaging, as photothermal additives or as complementary materials for energy conversion applications. Here, the synthesis of alkyl hydroxy-funtionalized, benz[*cd*]indole-donor capped squaraine dyes using the squaric acid or the dicyanomethylene-substituted squaraine acceptor unit is reported. In parallel synthesis, the hydroxy group is introduced directly on the dye-solubilizing alkyl side chains or coupled to the aryl part of the donor, and one or two functional linkers are attached. The hydroxy-functionalized dyes are then esterified with carboxyl groups attached to silica nanoparticles, a meltable polymer and a fullerene electron acceptor. Properties of the resulting hybrid material and organic conjugates demonstrate application merits of covalent bonding over blending for targeted photoinduced emission, heat and charge transfer reactions using near-infrared squaraine dyes.



[1] Haishima, Y.; Kubota, Y. Manseki, K.; *J. Org. Chem.* **2018**, *83*, 4389–4401.

[2] Wang, B.; Fan, J.; Sun, S. *Dyes and Pigments* **2010**, *85*, 43–50.

[3] Khopkar, S.; Shankarling, G. *Dyes and Pigments* **2019**, *170*, 107645.

[4] Karpenko, I. A.; Collot, M.; Richert, L.; Valencia, C. *J. Am. Chem. Soc.* **2015**, *137*, 405–412.

[5] Saikiran, M.; Sato, D.; Pandey, S. S. *Bioorg. Med. Chem. Lett.* **2017**, *27*, 4024–4029.

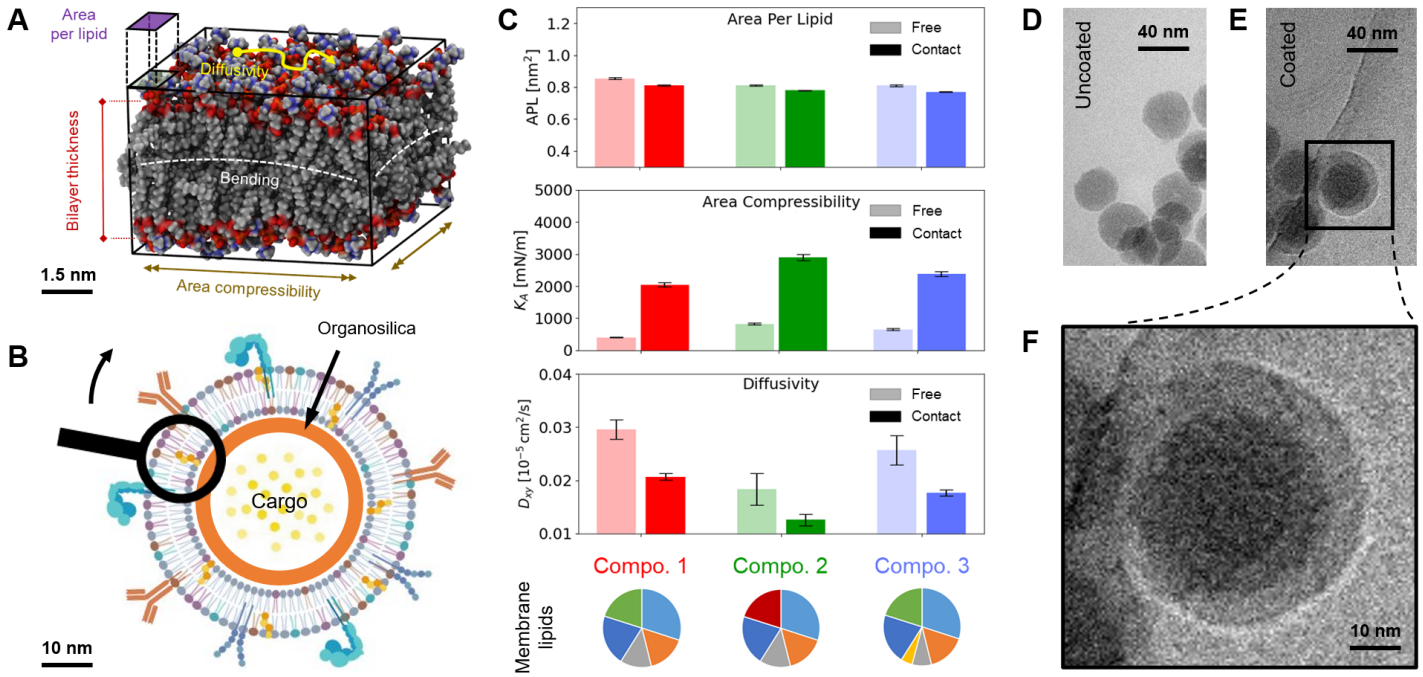
Towards Highly Specific Theranostics via Engineered Nanoparticles Mimicking Extracellular Vesicles: Focus on Envelope Dynamics

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Extracellular vesicles (EVs) are natural nanoscale carriers that mediate intercellular communication through the selective packaging and delivery of bioactive cargo. Their intrinsic tissue-recognition capacity makes them compelling templates for targeted therapeutic delivery, diagnostic imaging, and theranostic applications. However, EV biodistribution is governed by a complex interplay of surface proteins, glycans, lipid membrane composition, membrane curvature, and envelope dynamics (Fig. A), which together control recognition, stability, deformability, and diffusion through extracellular matrices. Reproducing these properties in synthetic systems therefore requires identifying minimal EV features that can be implemented in a controllable and clinically relevant formulation.

Within the MIMIC-KeY project (www.mimickey.eu), bone-tissue targeting was selected as a proof of concept for lysosomal bone metabolic disease, where selective bone delivery could enhance therapeutic efficacy while reducing systemic exposure. We developed EV-mimicking nanoparticles composed of a breakable organosilica core for payload encapsulation and controlled release, surrounded by a single-stack lipid bilayer envelope designed to host targeting proteins (Fig. B). Coarse-grained Martini molecular dynamics simulations were used to compare lipid compositions and quantify how compositional changes and contact with the organosilica core modulate the structural, mechanical, and dynamical properties of the lipid envelope. (Fig. C). Analysis of local membrane dynamics provided high-resolution fingerprints linking intra-membrane mobility to global envelope behavior. Cryo-TEM confirmed scalable synthesis of lipid-coated organosilica nanoparticles with a single bilayer envelope (Fig. D-F). This work establishes a framework for engineering minimal EV-mimicking nanocarriers with tunable envelope properties.

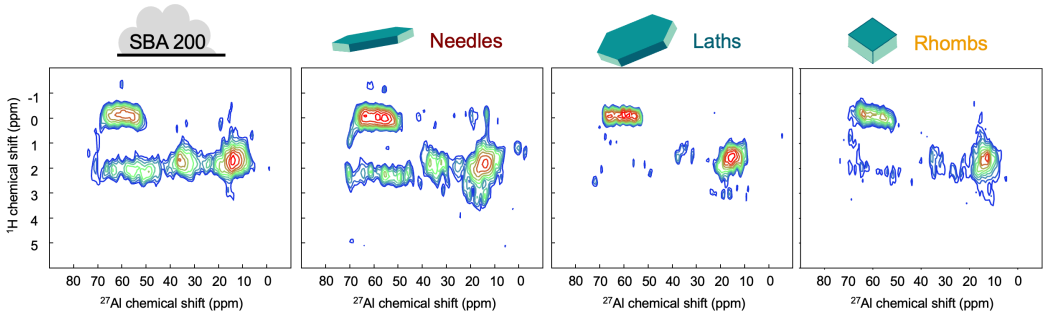


Investigating Facet-Dependent Surface Site Populations on γ-Alumina Morphologies and Their Influence on Transition Metal Immobilisation

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γ-Alumina (γ-Al_2O_3) is a cornerstone material in heterogeneous catalysis, widely utilised both as an active catalyst and as a support for transition metals.[1] The reactivity and selectivity of these systems are intrinsically governed by the local coordination environment of the surface aluminium atoms and hydroxyl groups. While recent breakthroughs utilising state-of-the-art solid-state NMR (ssNMR) spectroscopy have successfully mapped the complex fingerprint of tetra- (Al_{IV}), penta- (Al_V), and hexacoordinated (Al_{VI}) protonated surface sites on γ-alumina,[2,3] a systematic understanding of how macroscopic crystal morphology dictates site distribution and subsequent metal grafting behaviour remains a frontier challenge in rational catalyst design.



In this work, different morphologies of γ-Al_2O_3 exposing distinct aspect ratios and facet expressions (needles, laths, and rhombs) were synthesised and evaluated by routine physicochemical characterisation. To precisely map the surface topologies, advanced high-field 1.2 GHz 2D ^{1}H-^{27}Al D-HMQC surface NMR was employed, revealing distinct population changes of the surface aluminium atoms across the three supports. To demonstrate how these facet-dependent environments steer catalyst design, an organorhenium precursor was immobilised onto each support. Crucially, comparative post-grafting ^{1}H-^{27}Al surface NMR analyses exhibit subtle, morphology-specific variations in the coordination fingerprints, indicating that the local anchoring pathways are modulated by the exposed facets. We will discuss how these crystal shapes influence the grafting process, alongside ongoing ^{1}H-^{13}C studies to precisely identify the anchored metal species.

[1] Academic Press, Advances in Catalysis, 2014, 57, 319–404.

[2] D. Gioffrè, P. Florian, T. Pigeon, P. Raybaud, C. Chizallet, C. Copéret, Journal of the American Chemical Society, 2025, 147, 6934–6941.

[3] L. A. Völker, J. Meyet, Z. J. Berkson, L. Rochlitz, J. A. van Bokhoven, C. Copéret, Journal of Physical Chemistry C, 2022, 126, 6351–6360.

Highly Selective Solar Driven Biomass Reforming Coupled with Hydrogen Evolution on Cu2O Artificial Leaf

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Climate change remains an urgent global challenge, driving the development of sustainable strategies to meet the increasing demand for clean energy. Solar energy represents particularly attractive for deep decarbonization as it can be directly converted into storable chemical fuels[1]. Inspired by natural photosynthesis on the leaves, artificial leaf systems aim to realize solar to chemical conversion through coupled reduction and oxidation reactions. Photoelectrochemical devices enable a pathway by integrating light absorption, charge separation, and surface catalysis on semiconductor[2]. Cuprous oxide (Cu2O) is a promising p-type semiconductor for solar-driven water splitting owing to its suitable band gap, strong visible light absorption and high theoretical photocurrent density[3]. Cu2O based photoelectrodes have been investigated for photoelectrochemical water splitting reaction to hydrogen evolution reaction (HER), with remarkable improvements in onset potential and stability through interfacial engineering and protective overlayers[4]. Meanwhile, biomass oxidation can produce valuable chemicals while reducing the energetic penalty of oxygen evolution. Glucose oxidation reaction (GOR) represents particularly appealing because it proceeds at lower potentials (0.1~0.4 V vs RHE) than oxygen evolution (1.23 V vs RHE)[5], and the oxidation products are widely used in pharmaceuticals, food additives, and agriculture.

Herein, we investigated AuPd as an electrocatalyst for GOR and achieved nearly 100% Faradaic efficiency and 100% selectivity toward gluconic acid. Owing to its favourable onset potential and ideal current density, GOR was coupled with HER on the Cu2O-based integrated artificial leaf device. Cu2O serves as the light absorber, while charge selective transport layers promote photogenerated carrier separation and directional transfer to catalytic interfaces. Under simulated one sun illumination, the device achieved 100% selectivity for both H2 and gluconic acid formation, producing 40.3 μmol·cm−2 H2 and 43.0 μmol·cm−2 gluconic acid in the first hour, indicating well photogenerated charge balanced and utilization. Characterizations and mechanism analysis suggested that the high photovoltage and reasonable charge transport architectures are critical for high efficiency coupling hydrogen evolution with glucose oxidation. This work highlights that the promising and sustainable pathway for achieving solar driven fuel generation and value-added chemical synthesis on the integrated sustainable artificial leaves.

[1] J. Kim, D. Hansora, and P. Sharma, Chem. Soc. Rev., 2019, 48, 1908.
[2] T. Faunce, S. Styring, and M. R Wasielewski, Energy Environ. Sci., 2013, 6, 1074-1076.
[3] C. Li, T. Hisatomi, and O. Watanabe, Energy Environ. Sci., 2015, 8, 1493-1500.
[4] L. Pan, Y.Liu, and L.Yao, Nat Commun., 2020,11, 318 .
[5] Y. Liu, X.Tao, and C. Huang. Nat Commun., 2026, 17, 4372.

Emerging Industrially Ready Bifunctional Imide Monomers for Sustainable High-Performance Materials: Beyond Bisphenols and PFAS

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[1]VALSYNTHESE SA

In recent decades, increasing regulatory pressure on high-performance polymer building blocks, particularly bisphenols and per- and polyfluoroalkyl substances (PFAS) for polymer applications, has driven the search for safer and more sustainable molecular alternatives.

Here we introduce a modular, industrially scalable platform of bifunctional imide monomers designed for the development of high-performance materials across a broad range of applications. These monomers combine structural versatility with excellent thermomechanical robustness, enabling fine-tuning of material properties within a unified molecular framework. Owing to their synthetic accessibility and growing industrial interest, these systems are advancing from laboratory development toward application testing and pre-commercial evaluation in relevant technological sectors.

In short, bifunctional imide monomers represent an emerging platform for next-generation high-performance materials, integrating design flexibility, thermal stability, and industrial scalability, and offering a promising modern and greener alternative to currently regulated chemical systems.

Polymer Brushes via Controlled Surface-initiated Polymerization

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Polymer brushes are defined as thin polymer films in which the individual polymer chains are tethered by one chain end to a solid interface.[1] Polymer brushes have great advances to tailor the chemical and physical properties in surface and interface engineering. Among those synthesis strategies, surface-initiated atom transfer radical polymerization (SI-ATRP) has been one of the most widely applied strategies to synthesize polymer brushes via controlled surface-initiated polymerization. In this approach, initiators are immobilized on a surface, followed by brush growth via the grafting-from method. This approach has advantages, including high grafting density, controllable brush thickness, and nanoscale adjustable thickness.[2]

Although traditional vinyl-based monomers have been widely investigated, the development of novel vinyl monomers with diverse architectures is expected to show unique properties and broaden the potential applications.[3] Here, we present a synthetic strategy to prepare polymer brushes with long side chains via SI-ATRP. Kinetic study demonstrated a well-controlled polymerization process. Polymer brushes thickness are adjustable by varying the polymerization time. The long side chains offer the opportunity to incorporate functional groups, widened the physicochemical properties of polymer brushes. This polymer brushes show potential applications in lubricants, optical materials, antifouling coatings, and wearable devices.

[1] Justin O. Zoppe, Nariye Cavusoglu Ataman, Piotr Mocny, Jian Wang, John Moraes, Harm-Anton Klok, *Chemical Reviews*, **2017**, 117, 1105-1318.

[2] Kuljeet Kaur, Sabrina Sant, Leon A. Smook, Sissi de Beer, Harm-Anton Klok, *Angewandte Chemie International Edition,* **2026**, 0:e07712.

[3] Christian W. Pester, Harm-Anton Klok, Edmondo M. Benetti, *Macromolecules*, **2023**, 56, 9915-9938.

Cutting-Edge XRD Approaches for Battery Materials Characterization

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The rapidly growing demand for high-performance rechargeable batteries has intensified the need for advanced materials characterization techniques. X-ray diffraction (XRD) plays a central role in elucidating the crystallographic structure and dynamic evolution of electrode and electrolyte materials, both in situ and in operando. This presentation showcases state-of-the-art XRD methodologies developed at Rigaku for comprehensive characterization of next-generation battery systems - from raw material screening to full-cell evaluation.

We highlight the capabilities of the Rigaku SmartLab diffractometer platform, equipped with high-flux X-ray sources, advanced optical components, and detectors offering superior energy resolution. These features enable highly sensitive operando studies of lithium-ion and all-solid-state batteries, allowing real-time tracking of phase transitions, lattice parameter evolution, and changes in electronic states during charge–discharge cycling. The use of both reflection and transmission geometries allows simultaneous investigation of cathode and anode materials in practical configurations such as laminated and coin cells. Additionally, temperature- and pressure-controlled sample environments provide valuable insights into thermally induced phase transformations and ion transport mechanisms.

Beyond conventional diffraction techniques, we explore total scattering and Pair Distribution Function (PDF) analysis, which extend structural characterization to disordered and amorphous systems - critical for understanding local structure in solid electrolytes such as $Li_7P_3S_{11}$ and argyrodite-type materials. Furthermore, integration with complementary techniques-including X-ray fluorescence (XRF), X-ray emission spectroscopy (XES), and X-ray computed tomography (XCT) - enables multi-scale characterization spanning atomic to macroscopic levels.

Case studies will illustrate key applications, including phase stability in layered NCM cathodes, local structural heterogeneity in sulfide electrolytes, and real-time monitoring of structural degradation in full battery cells. By combining high-resolution diffraction, operando analysis, and local structural probes, these advanced XRD-based approaches provide a powerful and versatile toolkit for accelerating the development and optimization of next-generation lithium- and sodium-ion batteries.

Integrated Solid-State Characterization of Pharmaceuticals Using XRD and DSC

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Solid-state characterization plays a critical role in pharmaceutical development, particularly in understanding crystal structure, polymorphism, and phase transitions that directly impact drug performance and stability. This presentation highlights the combined use of X-ray diffraction (XRD) and differential scanning calorimetry (DSC), as well as their integration in a simultaneous XRD-DSC approach, for comprehensive material analysis.

XRD is widely applied for qualitative and quantitative phase identification, crystallinity assessment, and crystal structure determination.

DSC complements XRD by providing insight into thermal behaviour, including melting, crystallization, glass transitions, and polymorphic phase transformations. However, standalone DSC analysis may face limitations in resolving complex or overlapping thermal events and lacks direct structural information.

To address these challenges, a combined XRD-DSC technique allows simultaneous structural and thermal measurements under identical conditions. This integrated approach enhances interpretation of phase transitions and polymorphic changes by correlating diffraction patterns with thermal signals in real time. It also reduces sample requirements, analysis time, and overall experimental cost while improving data reliability.

The presentation will demonstrate practical applications of this methodology, including characterization of tolbutamide. The benefits of simultaneous analysis for R&D and quality control workflows in the pharmaceutical industry will be discussed.

Overall, the integration of XRD and DSC, particularly in a combined XRD-DSC platform, represents a powerful and efficient strategy for advanced solid-state characterization of pharmaceutical materials.

Earth-Abundant Metal Oxide Cocatalysts on $BiVO_4$ for Value-Added Photoelectrocatalytic Oxidation of Biomass-Derived Platform Chemicals

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The European Union plans to reduce the fossil-dependent energy and chemical sectors by highlighting and funding carbon-neutral alternatives to meet its ambitious goal of making Europe the first climate-neutral continent by 2050. The coupling of photocatalytic value-added oxidation of biomass-derived platform chemicals with the hydrogen evolution reaction (HER) is a strategy to address both problems, as it provides a source for green hydrogen and carbon-neutral chemical feedstock. This project aims to design a photoelectrocatalyst for the oxidation of glycerol into value-added platform chemicals that can replace fossil-based chemicals, which are currently used in industry as chemical feedstock for processes such as adhesives, cosmetics and polymer production. Here, bismuth vanadate (BVO) is used as the photoabsorber in combination with cobalt oxide and nickel oxide as the cocatalyst for the oxidation reaction.

Understanding the role of Zr source in the mechanism of UiO-66 MOF nucleation and growth

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Metal-organic frameworks (MOFs) are solid materials, comprised of metal-containing nodes interconnected with organic linkers and thus forming highly porous crystalline structures. Tunability of the properties of MOFs, such as pores size, defectivity and affinity to various adsorbates, determines their potential applications in catalysis, gas storage and separation. However, understanding of the molecular-level processes underlying the mechanisms of nucleation and growth of MOFs remains insufficient, which considerably hinders the rational design of novel materials of this class as well as optimization and scale up of the existing ones.

In the present work, we focus on the mechanism of UiO-66 crystallization – a MOF based on $[Zr_6O_4(OH)_4]^{12+}$ oxo-clusters, interconnected by terephthalate linkers. Recent works unravel the role of the solvent and modulators in UiO-66 crystallization, demonstrating an efficient way to control the macroscopic properties of the MOF.[1,2] Meanwhile, the influence of the nature of the Zr source used for the synthesis on the reaction process remains underexplored. Using a combination of quasi-simultaneous *in situ* time-resolved XRD and Zr K-edge XAS we demonstrate that the nature of the Zr salt used for UiO-66 synthesis determines the pathway of the metal nodes formation, governing the crystallization rate and the properties of the product. Utilization of $ZrCl_4$ makes the nucleation proceed through the stage of hydrolysis of chlorinated Zr species (step IA), which slows down the formation of the Zr_6-clusters (step IIA) and eventually leads to larger 100 – 150 nm UiO-66 crystals (step IIIA). $ZrBr_4$ and ZrI_4 due to lack of zirconium-halogen binding tend to undergo rapid hydrolysis in the reaction media (step IB) leading to a fast Zr_6-clusters generation though oligomeric oxo-forms of Zr (step IIB) and resulting in significantly smaller (~30 nm) crystals of the product (step IIIB). $ZrO(NO_3)_2$ as a precursor determines instant formation of the Zr_6-nodes followed by their rapid assembling into the UiO-66 structure with even lesser crystal size (~10 nm). Giving important insights into the molecular mechanisms of UiO-66 crystallization, this work contributes to the rational synthesis of MOFs and thus targeted adjustment of their macroscopic properties.

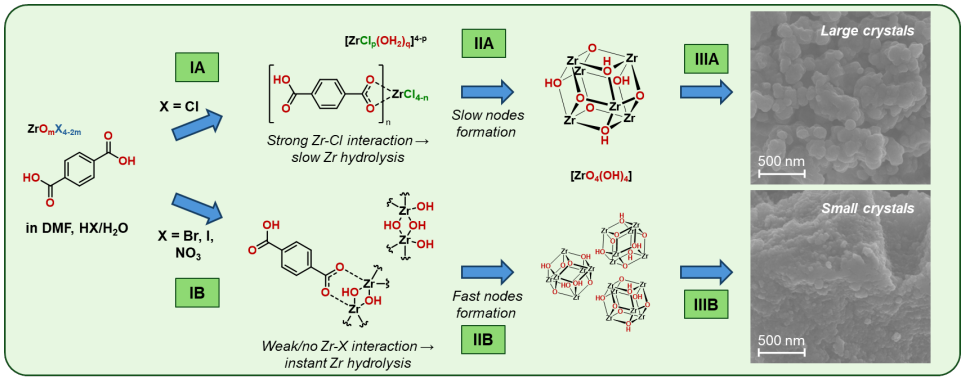


Figure 1. Proposed pathways of UiO-66 formation depending on the type of Zr precursor.

[1] O. O. Semivrazhskaya, D. Salionov, A. H. Clark, N. P. M. Casati, M. Nachtegaal, M. Ranocchiari, S. Bjelić, R. Verel, J. A. van Bokhoven, V. L. Sushkevich, *Small* **2023**, 19, 2305771.

[2] M. A. Artsiusheuski, N. P. M. Casati, A. H. Clark, M. Nachtegaal, R. Verel, J. A. van Bokhoven, V. L. Sushkevich, *Angew. Chem. Int. Ed.* **2025**, 64, e202415919.

Greener Depolymerization of ATRP Polymethacrylates Using Reducing Agents

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Chemical recycling to monomer has recently garnered increased interest for its ability to regenerate monomers from polymers at moderate temperatures by leveraging the functional end groups of CRP polymers for activation. Herein, we report the chemical recycling of ATRP-synthesized polymethacrylates, where high percentages of monomers (>80%) are successfully regenerated by addition of reducing agents. The reducing agent addition enables use of a greener solvent, anisole, the lowering of catalyst loading without significant reduction of overall conversion, and compatibility with a wide range of reducing agents (e.g. tin ethylhexanoate, glucose, and ascorbic acid). Altogether, we present a simpler and greener method to depolymerize polymethacrylates under mild conditions.

Neutral Ligands, Distinct Zeta Potentials: Consequences for Hafnium Oxide Nanoparticles Biodistribution

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Nanoparticles (NPs) play a crucial role in modern medicine, offering versatile platforms for targeted drug delivery, diagnostic imaging, and therapeutic applications due to their unique physico-chemical and surface properties [1-2]. Although the core composition of NPs dictates their functionality (magnetic, optical, or catalytic properties), in vivo performance and interactions with the biological environment are mainly dictated by their size and surface chemistry [3]. The ability to avoid detection by immune system is known as a stealth property and results in prolonged *in vivo* circulation of NPs. Several strategies have been developed to prepare stealth NPs, such as using polyethylene glycol-based (PEGylated) or zwitterionic (ZW) ligands. However, the head-to-head comparison of NPs stabilized with the same tightly binding group but with different neutrally charged ligand tails is still lacking to identify the best ligand for the preparation of stealth NPs for biomedical applications.

In this study, we used sub-5 nm HfO_2 NPs, as a model system, given their biocompatibility and established use in contrast-enhanced X-ray computed tomography and external-beam radiotherapy. We systematically compared three surface ligands with the same high-affinity nitrocatechol anchoring group but different terminal moieties: a short ethylene glycol oligomer, a 2 kDa PEG polymer, and a short zwitterion. Despite the neutral character of all ligand tails, only the long PEG chains yielded nanoparticles with a neutral zeta-potential, while both short ligands yielded NPs with a negative zeta-potential. This negative zeta-potential was then correlated with enhanced uptake by THP-1 macrophages *in vitro* and short circulation times *in vivo* in zebrafish larvae (Figure 1). In contrast, HfO_2 NPs stabilized with long PEG chains largely escaped detection by the phagocyte system. They exhibited prolonged circulation and extravasation in the zebrafish larva model, highlighting their promise for future targeted nanomedicine delivery.

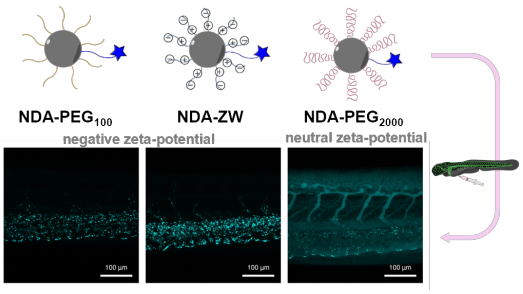


Figure 1. Three different surface ligands NDA-PEG100, NDA-ZW and NDA-PEG2000 were used to stabilize HfO2 NPs. Negative zeta-potential of NPs stabilized with short ligands resulted in rapid clearance of NPs from circulation of zebrafish larvae, while neutral zeta-potential of NPs capped with long PEG chains resulted in prolonged circulation and extravasation to surrounding tissues.

[1] Patra et al., Journal of nanobiotechnology, 2018, 16, 71.
[2] Alivisatos, P. Nature biotechnology, 2004, 22, 47–52.
[3] Bilardo et al., Wiley Interdisciplinary Reviews: Nanomedicine and Nanobiotechnology, 2022, 14, e1788.

Schraps™: Circular Bioplastics from Rapeseed Presscake

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The need to substitute petrochemical-based plastics with bio-based ones is pressing, due to increasing environmental concerns (insufficient biodegradability, release of microplastics) and geopolitical tensions (exacerbating resource scarcity).

Rapeseed presscake is the residue from rapeseed oil extraction, a by-product commonly used as cattlefeed. NeoChemurgy GmbH has recently developed a proprietary process allowing to conveniently transform rapeseed presscake into an innovative kind of bioplastics, called **Schraps™**.

Depending on the processing conditions, **Schraps™** bioplastic can be made to be rigid, or soft and flexible (*Figure 1*), moreover it possesses intrinsic fire-resistance and self-extinguishing properties. Possible fields of application range from packaging to construction panels.

Schraps™ bioplastics can be recycled in a way similar to conventional thermoplastics. Last but not least, their fabrication is environmentally friendly, energy-efficient, and results in materials that are biodegradable, even compostable.

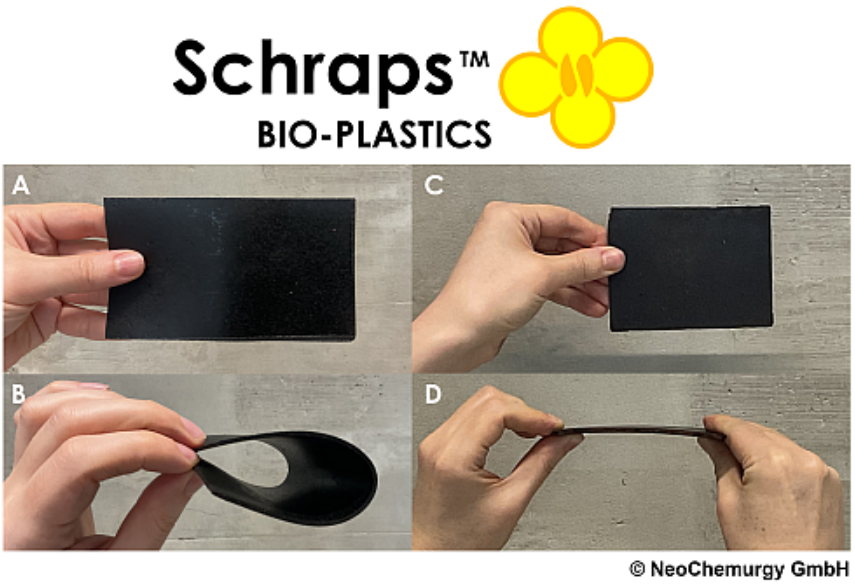


Figure 1. Samples of **Schraps™** bioplastics: flexible (A,B) and rigid (C,D).

Phyter™: Bio-based fire-retardants from rapeseed presscake

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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]. Rapeseed is 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, 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 into high-added value products such as **Phyter™**, a family of bio-based fire-retardants developed by NeoChemurgy GmbH.

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.

[1] J. A. Maga, Journal of Agricultural and Food Chemistry, **1982**, *30*, 1–9.

Towards a Controlled Introduction of Oxygen Vacancy to Metal Oxides

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The precise engineering of the surface of heterogeneous catalysts is crucial for the development of highly active and stable materials.[1] A promising alley to tune the catalytic activity of the important metal oxide-based catalysts is the introduction of vacancy defects into the materials.[2-3] Conventional methods to introduce vacancy defects into metal oxides typically involve harsh conditions, such as elevated temperatures, reactive atmospheres or plasma treatments.[4-6] This often leads to a variety of different defect sites in the materials that are challenging to quantify or analyze precisely. Characterization of the formed vacancies has proven difficult and is often controversially discussed.[7] To improve our understanding of defect-activity relationships and develop better material-based catalysts for better control over the vacancy formation is needed.

This poster describes our recently developed approach to introduce vacancies into transition metal oxides using a mild and controlled reaction. Our method further allows convenient quantification of the formed vacancies. EPR spectroscopy was employed to characterize the formed vacancies. The modified materials were then tested for epoxidation catalysis and compared to their defect-free analogues to evaluate the influence of the defects on catalytic performance. We demonstrate a correlation between the catalytic activity and distinct structural signatures of the formed vacancies. Our results thereby provide insight into structure-activity relationships for defective metal oxide based heterogeneous catalysts. This may open new possibilities for an improved defect engineering of metal oxide catalysts for future applications.

[1] I. Surin, Q. Yang, F. Krumeich, M. Agrachev, T. Otroshchenko, V. A. Kondratenko, E. V. Kondratenko, J. Pérez-Ramírez, *Chem. Catalysis,* **2025,** 5, 1, 101165.

[2] C. Xie, D. Yan, H. Li, S. Du, W. Chen, Y. Wang, Y. Zou, R. Chen and S. Wang, *ACS Catal*., **2020**, 10, 11082-11098.

[3] P. L. Gai-Boyes, *Catal. Rev. - Sci. Eng.*, **1992**, 34, 1-54.

[4] L. Xu, Q. Jiang, Z. Xiao, X. Li, J. Huo, S. Wang, L. Dai, *Angew. Chem. Int. Ed*., **2016**, 55, 5277-5281.

[5] Y. Kuwahara, Y. Yoshimura, K. Haematsu, H. Yamashita, *J. Am. Chem. Soc.*, **2018**, 140, 29, 9203-9210.

[6] G. Ou, Y. Xu, B. Wen, R. Lin, B. Ge, Y. Tang, Y. Liang, C. Yang, K. Huang, D. Zu, R. Yu, W. Chen, J. Li, H. Wu, L.-M. Liu, Y Li. *Nat. Commun.*, **2018**, 9, 1302.

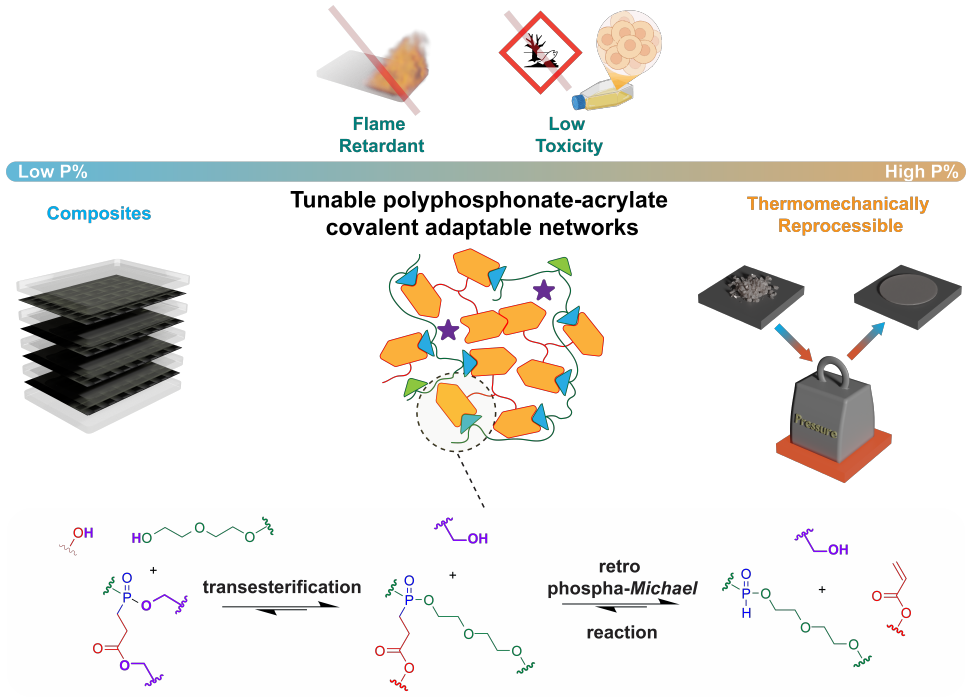
[7] T. J. Frankcombe, Y. Liu, *Chem. Mater.*, **2023**, 35, 5468-5474.

Challenging the Inertness of P–C Bonds: Reversible Phospha–*Michael* Chemistry in Dynamic Thermosets

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Carbon–phosphorus (P–C) bonds are generally regarded as chemically robust and effectively permanent once incorporated into polymer networks. Here, we demonstrate that phospha–*Michael*-derived P–C linkages can undergo thermally activated exchange within crosslinked polyphosphonate–acrylate thermosets, establishing dynamic P–C covalency as a previously unexplored mechanism for network rearrangement and covalent adaptable network behavior [1]. Polyphosphonate macromonomers were reacted with multifunctional acrylates to produce phosphorus-containing thermosets with tunable compositions and properties [2]. Evidence from model compounds, spectroscopy, stress-relaxation experiments, and network reprocessing supports a retro-phospha–*Michael* process operating alongside transesterification-mediated exchange. The resulting materials combine reprocessability with intrinsic flame retardancy, exhibiting self-extinguishing behavior and high limiting oxygen index values without external flame-retardant additives. The dynamic networks further enable repair, reshaping, and recovery of carbon fibers from composite materials. Acute aquatic toxicity testing following OECD guidelines provides an early *Safe-and-Sustainable-by-Design* perspective. This work establishes reversible phospha–*Michael* chemistry as a new dynamic covalent motif and introduces polyphosphonate–acrylate thermosets as a versatile platform for sustainable, flame-retardant, and recyclable polymer networks.



Dynamic P–C covalency and transesterification enables tunable flame retardant thermosets

[1] Damien Montarnal, Mathieu Capelot, François Tournilhac, Ludwik Leibler, *Science*, **2011**, 334, 965–968.

[2] Arvindh Sekar, Hermance Muller, Cédric Hervieu, et al., *Chemical Engineering Journal*, **2025**, 520, 165779.

Cs as a Probe to Elucidate the Nature of Specific Anchoring Sites on the Surface of Alumina Polymorph

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γ-Al_2O_3 is a premier catalyst support due to its high stability and porosity, yet a comprehensive description of its surface remains elusive [1]. While alkali metals (e.g., Li, K, Cs) are vital promoters for industrial processes like Fischer-Tropsch synthesis, the nature of their interaction with the support and the resulting anchoring sites are still debated [2]. To address these interconnected uncertainties, we propose using alkali metals as molecular probes. We focus specifically on Cs; its high atomic number (Z=55) facilitates HAADF-STEM imaging, while it is also an NMR-active nucleus enabling solid-state NMR (ssNMR**)**. This dual-characterization approach allows for a precise investigation of both the γ-Al_2O_3 surface and the newly generated alkali-promoted sites.

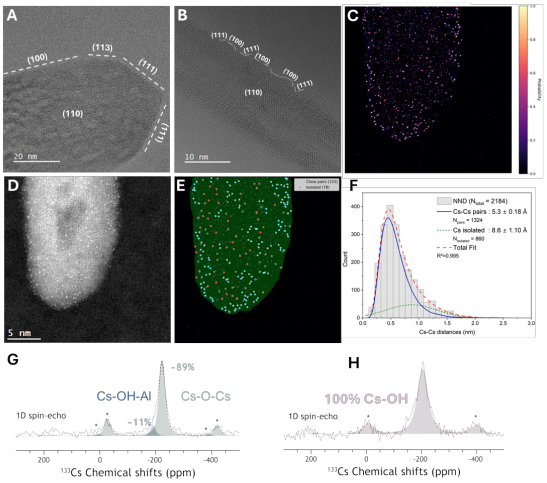


Figure 1: (A–B) HR-TEM and facet ID for γ-Al_2O_3 laths/needles; (C) Cs atom probability map; (D) HAADF-STEM of Cs-impregnated needle; (E) Identified Cs pairs (blue) and isolated atoms (red); (F) Cs–Cs distance histogram via NND; (G–H) ^{133}Cs ssNMR spectra of Cs-impregnated needles and laths.

Our approach utilizes morphologically defined γ-Al_2O_3 supports with distinct facets but identical bulk structures. γ-Al_2O_3 needles (Fig. 1A) exhibit pronounced nanofacetting with abundant (111)/(100) and (100)/(110) edge sites, host to specific anchoring sites, while laths (Fig. 1B) feature large, highly hydrated (111) terminations. Atomic dispersion of Cs (Fig. 1D) was achieved via IWI on both morphologies. Advanced TEM image processing [3] yielded a probability map (Fig. 1C) showing Cs preferentially forms pairs (5.3±0.2 Å), aligning with DFT-predicted pairing on needle edge sites. Isolated Cs atoms were also observed (8.6±1.1 Å); the higher standard deviation confirms a random distribution, unlike the well-defined pairs.^{133}Cs ssNMR confirmed two distinct species on needles (Fig. 1G), attributed to pairs and isolated atoms, whereas laths (Fig. 1H) show only one species near protons (2D ^{1}H-^{133}Cs ssNMR), reflecting higher hydroxylation and fewer edge sites. Ongoing TEM analysis aims to correlate these distributions with specific NMR signatures. These results demonstrate that combining STEM and NMR via Cs probes reveals morphology-dependent structural signatures, clarifying both the γ-Al_2O_3 surface and alkali anchoring sites.

[1] R. Prins, *Journal of Catalysis*, **2020**, 392, 336-346

[2] W. Liao *et al*. *Chemical Society Reviews,* **2025**, 54, 4164-4182

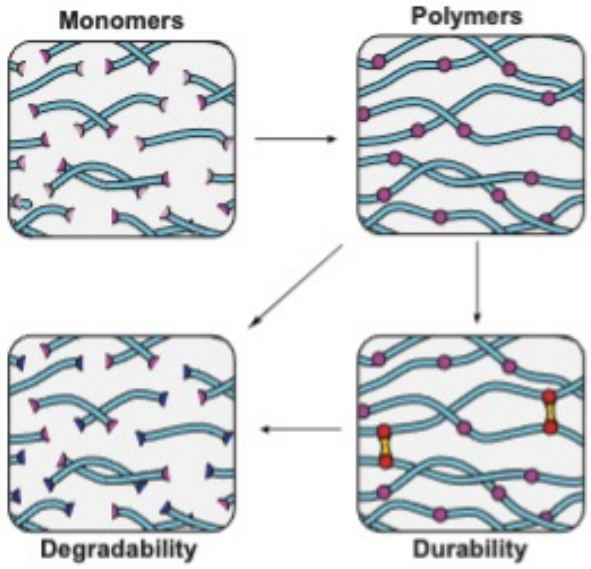
[3] S. Berg, S *et al. Nature Methods,* **2019**, 16, 1226–1232

Thioimidate-Based Polymers for Bridging Durability and Degradability

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The accumulation of plastic waste in landfills has raised concerns regarding its environmental impact and long-term sustainability.[1] While on-demand degradability of plastics is achievable through the incorporation of labile bonds, these bonds are disadvantageous when incorporated into plastics with long-term usage leading to their premature aging and loss of the material's properties over time.[2] Maintaining the properties of plastics throughout their lifetime is as important as degrading them at the end of their life. Designing a material with both high durability over long timescales and good degradability at any stage would be of high interest to decrease the amount of plastic waste. To bridge this degradability—durability trade-off, we designed a new class of polymeric materials based on thioimidates that can be degraded on-demand in acidic environments, yet undergo a self-healing and self-reinforcement mechanism when natural degradation occurs over time Our polythioimidates (polyTIs) are accessible through a bifunctional monomer that carries iminiumthiolactones (ITL) on both sides. The high reactivity of this bis(ITL) monomer promotes fast polycondensation with small aliphatic and aromatic amines or higher molecular weight polymers alike, essentially acting as a chain extender. The polymers synthesized with this building block showed good thermal stability up to 170 °C and tunable thermomechanical properties, while their on-demand degradation is achieved in aqueous HCl. The mechanical properties of the generated polyTIs are currently being investigated as well as how long-term degradation can be mitigated through the unique ITL-based self-healing and self-reinforcing mechanism. We believe that the molecular features of the presented polyTI materials can extend the lifetime of plastic materials while enabling on-demand degradation and hence may pave the way to more sustainable plastics and help reduce plastic waste.



[1] Roland Geyer, Jenna R. Jambeck, Kara Lavender Law, *Science Advances*, **2017**, 3, e1700782.

[2] L.C.E. Struik, *Polymer Engineering and Science*, **1977**, 17, 165-173.

Drug-carrier interactions in local antibiotic therapy with calcium sulphate: in situ time□resolved X-ray diffraction study

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Treating infections in orthopaedic and trauma surgery remains a significant challenge, requiring novel and effective therapeutic solutions. Local antibiotic therapy offers targeted treatment of bone and joint infections while limiting systemic toxicity. [1,2] Calcium sulfate ($CaSO_4$) is widely used as a resorbable carrier and is compatible with multiple antibiotics. The present study investigates the molecular interactions and controlled uptake mechanisms of antibiotic-loaded $CaSO_4$ carriers.

Drug-dependent uptake and hydration mechanisms of antibiotic-loaded $CaSO_4$ were conducted for commonly used antibiotics (tobramycin [3], vancomycin [2,3], and ceftriaxone [4]) via in situ time□resolved powder X□ray diffraction (PXRD). The final matrix microstructure and drug distribution were characterized by X□ray micro-CT and SEM-EDX.

Kinetic analysis revealed antibiotic-specific transformation rates with ceftriaxone and vancomycin, showing faster phase transition, with maximum rate constants of 4.5 and 4.0 $\%\cdot min^{-1}$ and complete transformation within 100 min, comparable to unloaded $CaSO_4$. In contrast, tobramycin reduced the maximum rate constant to 0.2 $\%\cdot min^{-1}$ within the longest transformation time of 2800 min. XCT showed that ceftriaxone has the strongest impact on pellet-scale morphology with a highly inhomogeneous pore distribution. SEM-EDX confirmed antibiotic-dependent crystal morphologies and localized drug distribution within high-density regions.

These findings demonstrate antibiotic-specific drug-carrier interactions: vancomycin primarily through extended hydrogen-bonding networks, ceftriaxone through Ca^{2+} complexation, and tobramycin through electrostatic adsorption complemented by H-bonding. This molecular□level framework for drug-carrier interactions supports the advancement of local antibiotic therapy and has direct implications for improving and optimizing infection control.

[1] Gramlich, Y., T. Johnson, M. Kemmerer, G. Walter, R. Hoffmann and A. Klug (2020), Knee Surg. Sports Traumatol. Arthrosc. 28(9): 2823-2834.
[2] Wahl, P., M. Guidi, E. Benninger, K. Ronn, E. Gautier, T. Buclin, J. L. Magnin and F. Livio (2017), Bone Joint J. 99-B(11): 1537-1544.
[3] Maale, G. E. Eager, J. J. Mohammadi, D. K. Calderon, F. A. (2020), Eur J Drug Metab Pharmacoki-net. (4)45, 547-555.
[4] Wahl, P., K. Rönn, M. Bohner, L. A. Decosterd, C. Meier, M. Schläppi, S. Festa, E. Gautier, (2018), J. Bone Joint Infect. 3(4), 212-221.

Synthesis of Stimuli-Responsive ABA Triblock Copolymer Hydrogels Utilizing Metal-Coordination

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ABA triblock copolymers have attracted significant interest due to their strong mechanical properties and re-processability. In aqueous systems, triblock copolymers that contain a water-soluble central block and hydrophobic outer blocks can self-assemble into hydrogels without permanent crosslinking. [1] Such materials can exhibit self-healing properties, enhancing their durability and service life. By introducing functional groups capable of stimuli-responsive physical crosslinking (e.g., hydrogen bonding or metal-ligand complexation), responsivity to factors such as pH and temperature can be imparted to hydrogels. These adaptive materials are promising for applications including biosensing, injectable materials, and controlled drug delivery. [2]

This project aims to utilize Reversible Addition-Fragmentation chain Transfer (RAFT) polymerization to develop ABA triblock copolymers that can undergo a sol-gel transition upon changes in environmental stimuli. The designed polymer contains a water-soluble middle block and functional groups capable of metal-coordination in the end blocks. Our preliminary results suggest that the developed polymer can form a pH-responsive hydrogel upon the introduction of metal ions. Current work is being carried out to understand the influence of metal-ligand interactions upon the hydrogel's rheological and mechanical properties.

[1] R. R Taribagil, M. A Hillmyer and T. P. Lodge, Macromolecules, 2010, 43, 5396-5404

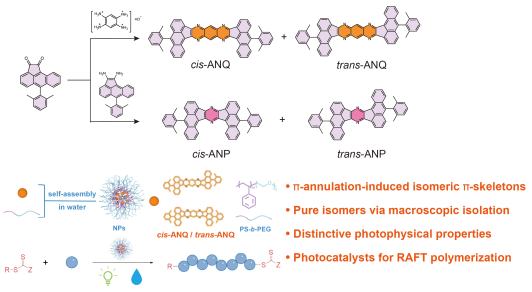
[2] H. Yin, F. Liu, T. Abdiryim and X. Liu, ACS Materials Letters, 2023, 5, 1787-1830

Elegant Strategies for Isolating Cis- and Trans-Isomers of Large π-Annulated N-Embedded Polycyclic Aromatics and Their Photocatalytic RAFT Applications

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The separation of pure stereoisomers and the elucidation of the relationship between their structures and properties remains major scientific challenges. Herein, we report the facile synthesis and isolation of pure *cis*- and *trans*-isomers of large π-annulated, N-embedded polycyclic aromatics via condensation reactions of aceanthrenequinone. A judiciously designed precursor, 6-(2,6-dimethylphenyl)aceanthrylene-1,2-dione, readily undergoes Schiff-base cyclocondensation with 1,2,4,5-benzenetetramine to produce the *cis*- and *trans*-isomers of ANQ, respectively. Moreover, this diketone can be converted into its corresponding diamine, 6-(2,6-dimethylphenyl)aceanthrylene-1,2-diamine. Both precursors react in a similar way to yield the *cis*- and *trans*-isomers of ANP, respectively. The observed *cis–trans* isomerism arises from the presence of the protruding fused benzene rings of the aceanthrene moiety. These isomers show a large difference in dipole moment and consequently, a substantial variation in retention factor (R_f). This makes them easy to purify on a macroscopic scale using standard column chromatography, and to characterize according to their ^{1}H NMR spectra. Depending on the nature of the linkers and molecular configurations, they show distinctive electronic absorption and emission features, solvatochromic behaviors, and photoluminescence quantum yields. TD-DFT calculations reveal significant variations in the electron density distribution between the *cis*- and *trans*-configurations, leading to substantial changes in the character of the optically active electronic transitions. Notably, both ANQ-isomers further self-assemble into water-soluble photocatalytic polymer nanoparticles that efficiently drive visible-light-mediated reversible addition-fragmentation chain transfer (RAFT) polymerization.



Interfacial Electric Field Regulation by 2D Au Mesh Interphase for Stable Zn Metal Anodes

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Aqueous Zn metal batteries are attractive for large scale energy storage because they combine the intrinsic safety of aqueous electrolytes with the high capacity, low cost, and natural abundance of Zn. Their practical application, however, is still limited by the poor reversibility of the Zn metal anode. During repeated plating and stripping, Zn deposition is often spatially nonuniform, which leads to rough deposits, dendritic or porous growth, dead Zn accumulation, and severe parasitic reactions at the Zn electrolyte interface. These problems originate from localized charge transfer and uneven Zn^{2+} supply during cycling, indicating that stabilization of the reactive interface is essential for durable Zn metal anodes.

Here, we design an Au Mesh Interphase on the Zn anode to regulate the interfacial electric field and spatial distribution of interfacial reactions. The interphase consists of a continuous two dimensional Au aerogel network with an open mesh structure. Its laterally connected conductive framework promotes electron redistribution across the Zn surface, extending charge transfer from localized regions to a broader interfacial area. At the same time, the open network preserves ion accessibility throughout the interface, enabling more uniform Zn^{2+} transport and alleviating concentration polarization near the electrode surface. Through this dual regulation of electron and ion pathways, the Au Mesh Interphase shifts Zn plating and stripping from a localized mode toward a more spatially distributed and controllable process.

This interfacial design provides a new strategy for stabilizing Zn metal anodes by coupling electric field regulation with sustained ion access. The work also offers mechanistic insight into the role of interfacial reaction fields in governing Zn deposition behavior and suggests a broader route for interface engineering in aqueous metal batteries.