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MaP | Competence Center for Materials and Processes

MaP Graduate Symposium 2024

and MaP Award Final

Symposium Booklet

MaP Doctoral School

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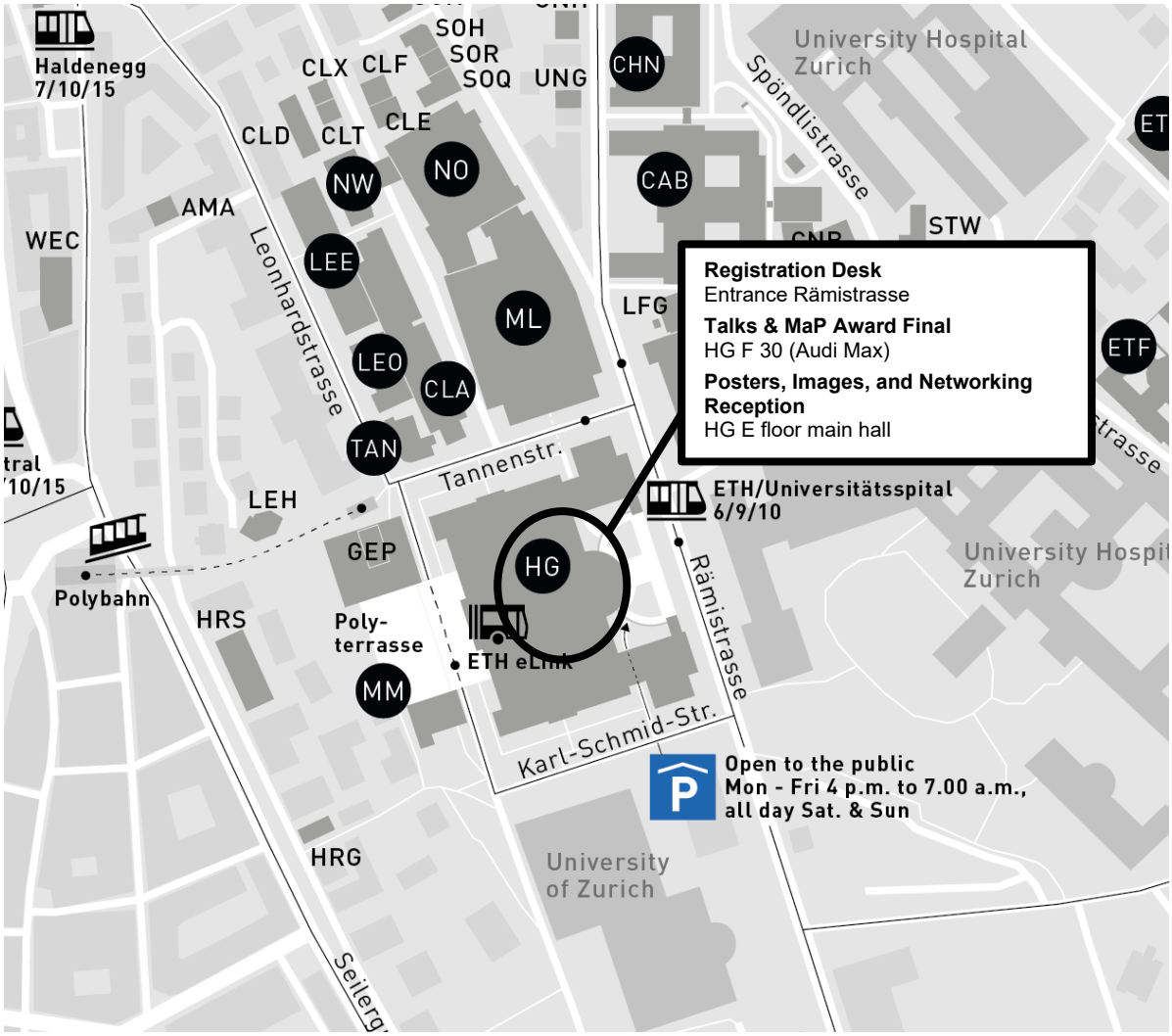

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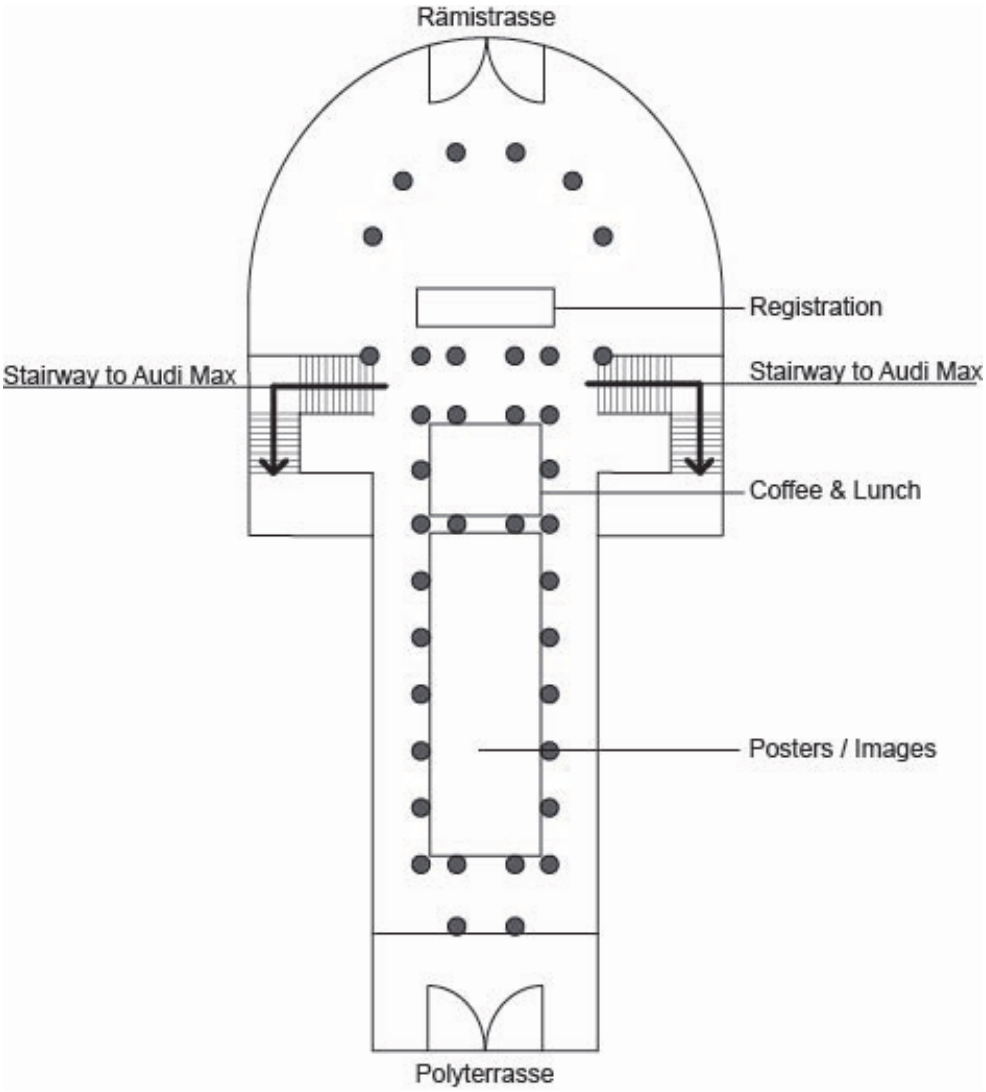

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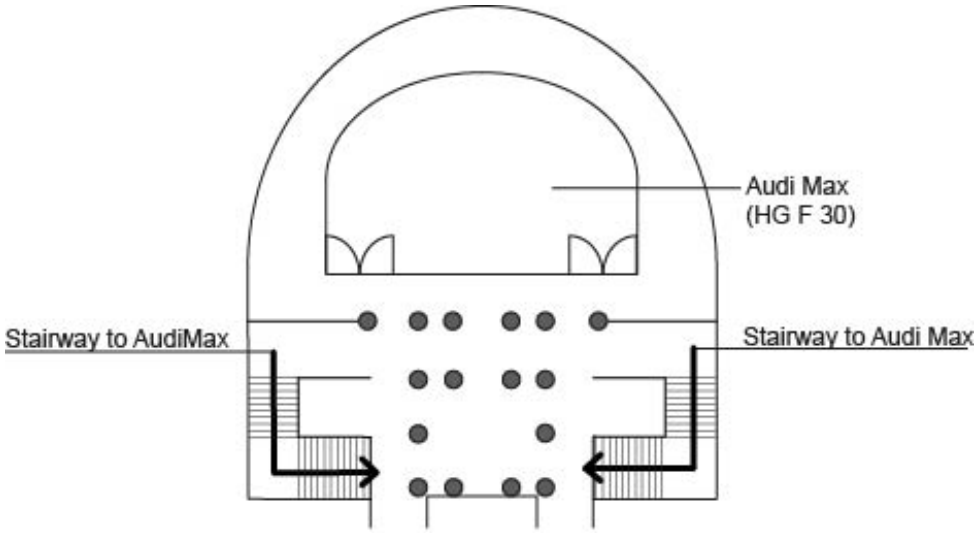

Programme

08.00	*Registration*	HG Entrance Hall
08.30	Opening Remarks	Audi Max
08.45	**Sara Svanberg**, *Bioanalytics Group, D-BSSE* Tooth-on-a-Chip: Biomaterial and Drug Testing Using a Dental in vitro Platform	Audi Max
	Johanna Byloff, *Nanometallurgy, D-MATL*, *Empa*: From Webb to Wrist: Adapting Space Sunshields for Everyday Electronics	
	Nicolas Rospars, *Multifunctional Materials, D-MATL:* Building an Ideal Interphase on Lithium Metal for Next Generations Batteries	
	Virginie de Mestral, *Computational Nanoelectronics, D-ITET:* Ab Initio Modelling of the Electro-Optical Properties of Barium Titanate	
09.35	One-minute Poster Pitches, Part I	Audi Max
10.05	*Coffee Break* Poster Session I + Image Gallery	HG Main Hall
11.00	**Styliani Afroditi Mountaki**, *Polymeric Materials, D-MATL:* Open-air Chemical Recycling: Fully Oxygen Tolerant ATRP Depolymerization	Audi Max
	Alexander Jessernig, *Nanoparticle Systems Engineering, D-MAVT:* Early Detection and Monitoring of Anastomotic Leaks via Naked Eye-readable, Non-electronic Macromolecular Network Sensors	
	Eva Zunzunegui Bru, *Food and Soft Materials, D-HEST:* Universality in the Structure and Dynamics of Water Under Lipidic Mesophase Soft Nanoconfinement	
	Xueting Shen, *Soft Materials and Interfaces, D-MATL:* Modulating Microswimmers Locomotion with Internal Liquid Compartment	
11.50	One-minute Poster Pitches, Part II	Audi Max
12.20	*Lunch* Poster Session II + Image Gallery	HG Main Hall

(continued)

MaP Award 2024		
14.00	**Dr. Xavier Aeby**, *Multifunctional Materials, D-MATL:* Development of Materials and Manufacturing Processes for Sustainable Printed Electronics	Audi Max
	Dr. Hamed Almohammadi, *Food and Soft Materials, D-HEST:* Control of Colloidal Self-Assembly by Liquid-Liquid Crystalline Phase Separation	
	Dr. Thaylan Pinheiro Araújo, *Advanced Catalysis Engineering, D-CHAB:* Design of Promoted Reducible Oxide Catalysts for Green Methanol Synthesis	
	Dr. Remo Schäppi, *Renewable Energy Carriers, D-MAVT:* Fuel from Sunlight and Air – Demonstration, Automation, and Parameter Analysis	
15.30	*Coffee Break*	HG Main Hall
16.00	**Maria Nefeli Antonopoulou***, Polymeric Materials, D-MATL*: Acid-triggered Radical Polymerization of Vinyl Monomers	Audi Max
	Davide Pecchio, *Mesoscopic Systems, D-MATL:* Ultrafast Laser Induced Magnetic Relaxation in Artificial Spin Ices	
	Valentin Gantenbein, *Multi-Scale Robotics, D-MAVT:* Microrobotic Superstructures for Transport and Delivery of Magnetic Micromachines	
	Jiuke Chen, *Advanced Fibers, D-MATL:* The Role of Phosphorus Flame Retardants in Mechanical Recycling of PET	
	Dominik Zürcher, *Biochemical Engineering, D-CHAB:* Real-time Observation of Protein Aggregation at Liquid-Liquid Interfaces in a Microfluidic Device	
	Mary Jialu Chen, *Composite Materials and Adaptive Structures, D-MAVT:* Manufacturing and Characterization of a Novel Composite Heart Valve Prosthesis	
17.15	Industry Presentations	Audi Max
17.30	Idea Pitch for a Novel Transdisciplinary Format Election MaP Student Representative	Audi Max
17.45	Award Ceremony	Audi Max
18.00	*Networking Apéro Riche*	HG Main Hall

Abstracts of Talks

Session 1: 08.45 – 09.35

Chair: Prof. Robert Katzschmann (D-MAVT)

Svanberg Sara **CONFIDENTIAL**

Tooth-On-a-Chip: Biomaterial and Drug Testing Using a Dental in Vitro Platform

Sara Svanberg [1], and Petra S. Dittrich [2]

[1] Bioanalytics Group, D-BSSE, ETH Zurich

Byloff Johanna (non-confidential)

From Webb to Wrist: Adapting Space Sunshields for Everyday Electronics

Johanna Byloff [1, 2], Pierre-Olivier Renault [3], Damien Faurie [4], S. Altaf Husain [4], Thomas E. J. Edwards [2], Daniele Casari [2], Barbara Putz [2, 5]

[1] Nanometallurgy, D-MATL, ETH Zurich
[2] Nanomechanics, Advanced Materials and Surfaces, Empa
[3] Institut PPrime, Sciences des Matériaux, Université de Poitiers
[4] LSPM - CNRS, Université Sorbonne Paris Nord
[5] Institute for Functional and Structural Ceramics, Montanuniversität Leoben

Metal thin films on polymers are a promising avenue for flexible electronics and space applications. However, key challenges that currently prevent widespread deployment include mechanical failure during use, material restrictions, and limited recyclability. In the Al-Polyimide (PI) system, primary material in the James Webb telescope sunshield, favorable adhesive properties are attributed to an amorphous Al-O-C interlayer [1-2] (IL, 5 nm) between metal film and substrate. Through a combined atomic layer (ALD, 5 nm Al_2O_3) and physical vapor deposition (PVD, 150 nm Al) setup, we are able to mimic this interlayer artificially. Different Al/Al_2O_3 bi-layer sample geometries were deposited on polyimide and subjected to uni- and equi-biaxial tensile loading [3] and unloading with in-situ film stress (X-ray diffraction) and electrical resistivity measurements (four-point probe) at synchrotrons BESSY-II and SOLEIL, respectively. The evolution of Al film stress, width of the Al diffraction peak and electrical resistivity as a function of the applied strain and IL thickness could be determined. TEM and SEM analysis ascertained microstructure and post-mortem crack density, while adhesion energy was calculated via AFM analysis of tensile induced delaminations (buckles). The samples with artificial ALD interlayers exhibit reduced roughness and grain width in the PVD sputtered Al layer and higher adhesion energy, resulting in 50% improvement of electromechanical properties. This is possibly due favorable modifications of the PI substrate surface, showing that PVD film growth can be positively influenced by a preceding ALD step. As our combined ALD-PVD approach improves mechanical and interfacial properties of currently deployed thin film systems, they become more viable for widespread use in terrestrial and space applications.

[1] S. H. Oh, et al., Scr. Mater. 65, 5 (2011)
[2] L. Atanasoska, et al., J. Vac. Sci. 5, 6 (1987)
[3] G. Geandier, et al., Rev. Sci. Instrum. 81 (2010

Rospars Nicolas **CONFIDENTIAL**

Building An Ideal Interphase On Lithium Metal For Next Generations Batteries

Nicolas Rospars [1] [2], Mohammed Srout [1], Chengyin Fu [1], Gaël Mourouga [1], Mounir Mensi [3], Andrea Ingenito [1]

[1] Battery Innovation Hub, CSEM Centre Suisse d'Électronique et de Microtechnique
[2] Multifunctional Materials, D-MATL, ETH Zurich
[3] X-ray Diffraction and Surface Analytics Platform (XRD-SAP), Chemical Sciences and Engineering, EPFL

de Mestral Virginie (non-confidential)

Ab Initio Modelling of the Electro-Optical Properties of Barium Titanate

Virginie de Mestral [1], Lorenzo Bastonero [2,3], Michele Kotiuga [3], Marko Mladenovic [1], Nicolas Marzari [2,3], Mathieu Luisier [1]

[1] Computational Nanoelectronics, D-ITET, ETH Zurich
[2] U Bremen Excellence Chair, Bremen Center for Computational Materials Science, University of Bremen
[3] THEOS, Department of Materials, EPFL

Silicon photonics integrated electro-optical modulators based on barium titanate (BTO) can greatly improve the bandwidth of telecommunication devices and help reduce their power consumption. The physics of the modulator rely on the so-called Pockels effect, where the optical refractive index of a material can be tuned by an applied electric field.

In order to fabricate high-performance BTO modulators, a precise understanding of the Pockels effect and of its dependence on crystal defects is required. For this, we developed a framework calculating the electronic and vibrational contributions to the Pockels tensor from first-principles using density functional theory (DFT), the modern theory of polarization, a finite-difference approach, and an electronic Hubbard correction. Additionally, dynamic instabilities associated with the room-temperature stable phase of BTO were stabilised thanks to a supercell construction, where atomic degrees of freedom were enabled along the soft phonon modes eigenvectors.

Compared to the standard perturbative approach, our method is low-symmetry friendly, scales with one less order of magnitude, and is compatible with all DFT exchange-correlation functionals. Here, we successfully reproduce the r_{13} and r_{33} coefficients of the ground state tetragonal BTO Pockels tensor. In contrast, the r_{51} tensor elements are strongly affected by vibrational contributions via the change in Raman polarizability, and optical phonon modes polarities and frequencies. We show that in particular, r_{51} increases as a function of titanium displacement towards the tetragonal high-symmetry configuration.

[publication in preparation]

Session 2: 11.00 – 11.50

Chair: Prof Andreas Güntner, (Human-centered Sensing, D-MAVT)

Mountaki Stella Afroditi CONFIDENTIAL

Open-Air Chemical Recycling: Fully Oxygen Tolerant ATRP Depolymerization

Stella Afroditi Mountaki [1], Richard Whitfield [1], Evelina Liarou [2], Nghia P. Truong [1], Athina Anastasaki [1]

[1] Polymeric Materials, D-MATL, ETH Zurich
[2] Department of Chemistry, University of Warwick

Jessernig Alexander (non-confidential)

Early Detection and Monitoring of Anastomotic Leaks via Naked Eye-readable, Non-electronic Macromolecular Network Sensors

Alexander Jessernig [1,2], Alexandre H.C. Anthis [1,2], Emilie Vonna [1], Jachym Rosendorf [4,5], Vaclav Liska [4,5], Jeannette Widmer [3] Andrea A. Schlegel [6], Inge K. Herrmann [1,2,7,8]

[1] Nanoparticle Systems Engineering, D-MAVT, ETH Zurich
[2] Particles-Biology Interactions, Department of Materials Meet Life, Empa
[3] Department of Surgery and Transplantation, Swiss HPB Centre, University Hospital Zurich
[4] Department of Surgery, Faculty of Medicine in Pilsen, Charles University
[5] Biomedical Center, Faculty of Medicine in Pilsen, Charles University
[6] Transplantation Center, Digestive Disease and Surgery Institute and Department of Immunity and Inflammation, Lerner Research Institute, Cleveland Clinic
[7] The Ingenuity Lab, University Hospital Balgrist, Balgrist Campus
[8] Faculty of Medicine, University of Zurich

Anastomotic leakage (AL) is the leaking of non-sterile gastrointestinal contents into a patient's abdominal cav-ity. AL is one of the most dreaded complications following gastrointestinal surgery, with mortality rates reach-ing up to 27% [1]. The current diagnostic methods for detecting anastomotic leaks are limited in sensitivity and specificity, and are only effective in advanced stages when the leak has fully developed and symptoms are evi-dent [2-4]. Since the timing of detection directly impacts patient outcomes, developing new, fast, and simple meth-ods for early leak detection is crucial. Here, we introduce a naked eye-readable, electronic-free macromolecu-lar network drain fluid sensor for continuous monitoring and early detection of AL at the patient's bedside. The sensor array comprises three different bio-inspired macromolecular network sensing elements, each tailored for selectivity towards the three major digestive enzymes (amylase, lipase, and protease) found in the drainage fluid during a developing AL. Upon digestion of the macromolecular network structure by the respective diges-tive enzymes, the integrated coloring agent produces an optical shift discernible to the naked eye. The diagnos-tic efficacy and clinical applicability of these sensors have been demonstrated using clinical samples from 32 patients undergoing gastrointestinal surgery, yielding a Receiver Operating Characteristic Area Under the Curve (ROC AUC) of 1.0. As there is currently no satisfactory diagnostic method for AL detection, this work has the potential to significantly contribute to improved patient outcomes through continuous monitoring and early, low-cost, and reliable AL detection.

[1] A. H. Choudhuri, et. al., Indian J Crit Care Med. 17 (5), 298–303 (2013)
[2] B. A. Messias, et. al., Scientific reports 10 (1), 1–8 (2020)
[3] D. E. Yeung, et. al., International Journal of Colorectal Disease 36, 1147–1162 (2021)
[4] A. Almeida, et.al., International Journal of Surgery 10 (2), 87–91 (2012)

Zunzunegui-Bru Eva (non-confidential)

Universality in the Structure and Dynamics of Water Under Lipidic Mesophase Soft Nanoconfinement

Eva Zunzunegui-Bru [1],Serena Rosa Alfarano [1], Patrick Zueblin [1], Hendrik Vondracek [2], Federica Piccirilli [2],[3], Lisa Vaccari [2], Salvatore Assenza [4],[5],[6], Raffaele Mezzenga[1],[7]

[1] Food and Soft Materials, D-HEST, ETH Zurich
[2] Elettra Sincrotrone Trieste, Italy
[3] Instituto Innovazione e Ricerca Tecnologica (RIT), Area Science Park, Trieste, Italy
[4] Condensed Matter Physics Center (IFIMAC), Universidad Autónoma de Madrid, Madrid, Spain
[5] Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain
[6] Instituto Nicolás Cabrera, Universidad Autónoma de Madrid, Spain
[7] D-MATL, ETH Zurich

Water under soft nanoconfinement features physical and chemical properties fundamentally different from bulk water; yet, the multitude and specificity of confining systems and geometries mask any of its potentially universal traits. Here, we advance in this quest by resorting to lipidic mesophases [1] as an ideal nanoconfinement system, allowing inspecting the behavior of water under systematic changes in the topological and geometrical properties of the confining medium [2], without altering the chemical nature of the interfaces. By combining Terahertz absorption spectroscopy experiments and molecular dynamics simulations, we unveil the presence of universal laws governing the physics of nanoconfined water, recapitulating the data collected at varying levels of hydration and nanoconfinement topologies. This geometry-independent universality is evidenced by the existence of master curves characterizing both the structure and dynamics of simulated water as a function of the distance from the lipid-water interface. Based on our theoretical findings, we predict a parameter-free law describing the amount of interfacial water against the structural dimension of the system (i.e. the lattice parameter), which captures both the experimental and numerical results within the same curve, without any fitting. Our results shed light onto the fundamental physics of water under soft nanoconfinement and provide a practical tool for accurately estimating the amount of non-bulk water based on structural experimental data [3].

[1] Assenza, S.; Mezzenga, R. Nat. Rev. Phys. 1, 551–566 (2019)
[2] Assenza, S.; Mezzenga, R. J. Chem. Phys. 148 (2018).
[3] Mezzenga, R. Front. Soft Matter. 3, 1324589 (2023).

Shen Xueting (non-confidential)

Modulating Microswimmers Locomotion with Internal Liquid Compartment

Xueting Shen [1], Minghan Hu [2], Yang Yao [3], Federico Paratore[1] and Lucio Isa [1]

[1] Soft Materials and Interfaces, D-MATL, ETH Zurich
[2] Robotics and Intelligent Systems, D-MAVT ETH Zurich
[3] Department of Chemistry, Uni Basel

Among the range of existing artificial microswimmers, colloidal clusters offer the possibility to tune geometry and composition, and hence propulsion, in a versatile way[1][2]. Achieving precise control over the locomotion of artificial microswimmers is essential in many aspects, including the development of materials with diverse applications, from targeted drug delivery to microrobotics. Here, we propose a novel approach to modulating the locomotion of such microswimmers, including their swimming speed and direction, while preserving their surface properties. Our approach involves two steps. First, by using microfluidic synthesis, we encapsulate ionic liquids of different concentrations within oil-filled PMMA microcapsules. Next, by employing sCAPA [3][4], we attach each microcapsule to a silica microparticle to form “dimer” microswimmers. We then investigate the self-propulsion of these microswimmers on top of transparent electrodes under AC electric fields in the kHz range and demonstrate the ability to precisely control the velocity and propelling direction of the microswimmers by tuning the amount of encapsulated ionic liquid. We hypothesize the addition of ionic liquids changes the bulk conductivity of the microcapsule without affecting its surface dielectric properties and in turn regulates the electro-hydrodynamic flows responsible for propulsion. The incorporation of ionic liquids in liquid-filled compartments offers a versatile platform to modulate self-propulsion in active colloidal systems with the potential for encapsulation of a diverse range of cargoes.

1] S Ni, L Isa and H Wolf. Soft Matter, 14, pp. 2978-2995 (2018)
[2] L Alvarez, MA Fernandez-Rodriguez, A Alegria, S Arrese-Igor, K Zhao, M Kröger and L Isa. Nature Communications, 12:4762 (2021)
[3] M Hu, X Shen, D Tran, Z Ma and L Isa. Journal of Physics: Condensed Matter, 35, 435101 (2023)
[4] S Ni, J Leemann, I Buttinoni, L Isa and H Wolf. Science Advances, 2(4), e1501779 (2016)

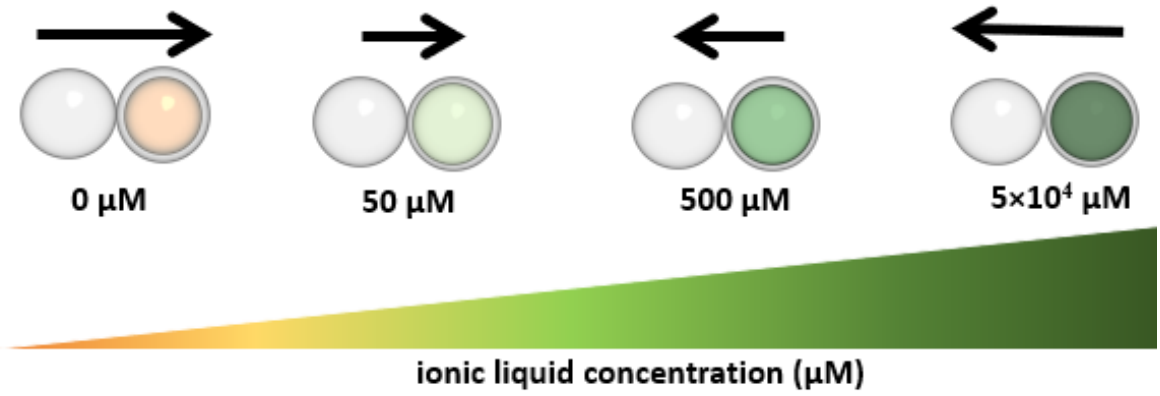

Figure. “Dimer” microswimmers with tunable swimming speed and direction regulated by the incorporation of different concentrations of the ionic liquid Trihexyltetradecylphosphonium in an oil-filled compartment. These microswimmers are composed of silica microparticle (white spheres) and poly(methyl methacrylate) microcapsule (colored) filled by hexadecane and varying concentrations of the ionic liquid. By altering the concentrations of ionic liquid, the swimming speed and direction under an AC field, as represented by the black arrows, changes.

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14.00– 15.30

Chair: Prof. Lucio Isa (Soft Materials and Interfaces, D-MATL)

Development of Materials and Manufacturing Processes for Sustainable Printed Electronics

Dr. Xavier Aeby

Multifunctional Materials, D-MATL, ETH Zurich

The development of internet-of-things for wearables, point-of-care testing or packaging, as an example, has given rise to a new generation of electronics that is characterized by a short service-life and a large quantity of devices produced. Today, a significant mismatch between the possible maximum lifespan and most common service-life of such connected devices exists. The service-life is typically measured in days, as opposed to years or even decades for the lifespan. This discrepancy is generating an exponentially increasing amount of electronic waste (e-waste). Unfortunately, the recovery and recycling of this e-waste is a tedious and expensive process with most of it ending up buried or discarded in landfills, potentially causing health and environmental risks. To mitigate e-waste generation and its associated environmental threats, new materials strategies are needed regarding electronics constituents, as well as a shift of paradigm regarding the key production metrics such as cost, industrialization and production throughput. Some of these metrics, for instance cost and throughput, have been widely investigated through the development of printed electronics. However, the use of sustainable or even biodegradable materials is still largely unexplored in this field, and their impact on devices' performance is rarely studied. Through the development of biodegradable materials and associated processes for electronics, it is aimed to propose an alternative to toxic materials, towards the safe disposal of e-waste.

Control of Colloidal Self-Assembly by Liquid-Liquid Crystalline Phase Separation

Dr. Hamed Almohammadi

Food and Soft Materials, D-HEST

Nucleation and growth (N&G) -the mechanism of forming a new thermodynamic phase- is one of the most important physical phenomena underlying gas-liquid, liquid-liquid, and solid-liquid phase separation. Understanding and controlling N&G have wide-reaching implications across various fields, from physics to material science, biology, and medicine. In principle, properties of newly emerged phases through N&G are determined by the interplay between thermodynamics and kinetics. In this talk, I will present an approach to control the properties of newly emerged phases through the N&G process in filamentous biocolloidal systems by disentangling the effects of kinetics from thermodynamics. I will first discuss the non-equilibrium features of filamentous colloidal systems. Next, I will discuss how understanding such features enabled us to present an approach to control properties, including shape, size, composition, orientation, structure, and formation time, in colloidal phases formed through the N&G process. Additionally, I will show the potential of our method to fabricate on-demand multicomponent heterogeneous colloidal systems. Lastly, I will discuss conceptual insights offered by our results that may help with addressing challenges in soft matter and biophysics fields and the practical implications of our approach to developing novel structural materials.

Design of Promoted Reducible Oxide Catalysts for Green Methanol Synthesis

Dr. Thaylan Pinheiro Araújo

Advanced Catalysis Engineering, D-CHAB

Methanol synthesis *via* thermocatalytic hydrogenation of carbon dioxide is a strategic route to enable the sustainable production of this vital commodity and energy carrier. However, the industrial implementation of this approach is limited by a lack of fundamental understanding of the catalytic materials used. To address this critical aspect, this thesis integrated precision catalyst synthesis, accurate catalytic evaluation, in-depth characterization, theoretical modelling, and kinetic studies to establish synthesis-structure-performance relationships for promising methanol synthesis catalysts based on reducible oxides, such as indium oxide (In_2O_3) and mixed zinc-zirconium oxides ($ZnZrO_x$). Through this holistic approach, the thesis establishes an atomic-level rationalization of In_2O_3 and $ZnZrO_x$ promotion by different metal promoters, offering key guidelines for the design of optimal systems. It was possible to overcome synthetic constraints by engineering multicomponent catalysts using flame spray pyrolysis, creating tailored catalyst architectures with superior performance. This approach led to the development of ternary Pd-In_2O_3-ZrO_2 systems with enhanced oxygen vacancy generation that display unparalleled methanol productivity and stability, as well as $ZnZrO_x$ systems with maximized surface area and density of catalytic ensembles that outperform benchmark catalysts attained by coprecipitation. Finally, a systematic investigation using ex situ and in situ electron paramagnetic resonance spectroscopy provides a means to characterize oxygen vacancies on In_2O_3- and $ZnZrO_x$-based catalysts, advancing understanding of this critical performance descriptor. The findings presented offer design criteria for the development of innovative and efficient catalytic technologies that can propel green methanol production at industrial scale.

Fuel from Sunlight and Air – Demonstration, Automation, and Parameter Analysis

Dr. Remo Schäppi

Renewable Energy Carriers, D-MAVT

This thesis reports on the technological demonstration under real field conditions of the entire process chain to drop-in fuels from concentrated sunlight and ambient air.

Crucial to this accomplished milestone is the design and integration of three thermochemical conversion units: A direct air capture unit for the co-extraction of CO2 and H2O directly from air, a solar redox unit performing the solar redox co-splitting of CO2 and H2O to produce a desired syngas mixture, and the gas-to-liquid synthesis unit converting the syngas to liquid methanol or hydrocarbon fuels. This thesis presents the components of the implemented process chain and shows the fully automated full day cyclic production of syngas suitable for either methanol or Fischer-Tropsch synthesis, demonstrating the stability and robustness of the system and producing the first methanol from sunlight and air via the thermochemical pathway. The entire solar fuel system is fully-automated based on real-time product gas analysis and feedback control loops, and can be further extended with an auto-optimisation scheme that executes online mass and energy balances to guide performance improvement. A parametric study of the main operational parameters (namely: reactor pressure, reduction-end and oxidation-start temperatures, CO2 and H2O mass flow rates) determines the influence on key performance indicators such as the fuel yield, molar conversion, and solar-to-fuel energy efficiency.

A dynamic grey box model of the redox reactor is developed for the purpose of further examining the dependence of reactor outputs to reactor inputs and investigating different operation procedures. Applying a simplified model to simulate a two and three reactor system that make continuous use of the incident solar power, allows the comparison and discussion of incorporating an additional reactor.

Session 3: 16.00 – 17.15

Chair: Prof Maksym Yarema (Chemistry and Materials Design, D-ITET)

Antonopoulou Maria-Nefeli (non-confidential)

Acid-Triggered Radical Polymerization of Vinyl Monomers

Maria-Nefeli Antonopoulou [1], Athina Anastasaki [1]

[1] Polymeric Materials, D-MATL, ETH Zurich

Reversible addition–fragmentation chain-transfer (RAFT) polymerization is one of the most versatile and robust controlled radical polymerization methods owing to its broad material scope and high tolerance to various functionalities and impurities. However, to operate RAFT polymerization, a constant supply of radicals is required, typically via exogenous thermal radical initiators that are not only challenging to transport and store, but also primarily responsible for termination and end-group heterogeneity. [1] Here we present an acid-triggered RAFT polymerization that operates in the dark and without any conventional radical initiator. Abundant acids (for example, sulfuric acid) are shown to have a dual role initiating and accelerating the polymerization. The polymers prepared have low dispersity and high end-group fidelity. The method is compatible with a wide range of vinyl monomers and solvents, and can be applied to the synthesis of well-controlled high molecular weight block copolymers, as well as to free radical polymerization.

[1] J. Chiefari, et al., Macromolecules 31, 5559–5562 (1998).
[2] A. Anastasaki et al. Nat. Synth 3, 347–356 (2024).

Pecchio Davide (non-confidential)

Ultrafast Laser Induced Magnetic Relaxation in Artificial Spin Ices

Davide Pecchio [1, 2], Sourav Sahoo [1, 2], Gavin M. Macauley [1, 2], Valerio Scagnoli [1, 2] and Laura J. Heyderman [1, 2]

[1] Mesoscopic Systems, D-MATL, ETH Zurich
[2] Multiscale Materials Experiments, Paul Scherrer Institute

Artificial spin ices (ASIs) are arrays of dipolar-coupled single-domain nanomagnets, arranged in suitable lattice geometries. These systems have played a pivotal role in exploring frustration, emergent magnetic monopoles and phase transitions [1]. In addition, their use is envisioned for memory applications, logic operations and reprogrammable magnonic crystals.
We demonstrate how the magnetic configuration of nanomagnets relaxes to a low-energy state within a few nanoseconds on exposure to a femtosecond laser pulse. The samples are made of densely-packed stadium-shaped permalloy nanomagnets placed on square and kagome lattices. Following ultrafast demagnetization, the magnetic moments of nanomagnets try to reconfigure themselves to minimize their total energy, striving to satisfy the dipolar interactions.
A square lattice was analyzed first, given its well-defined ground state, to assess the efficacy of the newly proposed methodology. The system is initially saturated in a high-energy state with an external magnetic field, then exposed to 100 fs laser pulses. The resulting magnetic configurations are imaged with MFM, showing that, above a certain threshold fluence, large (8x8 um2) ground state domains with Type I vertex configurations form (Fig. 1).
[1] S. H. Skjærvø, et. al., Nat. Rev. Phys. 2, 13 (2020)

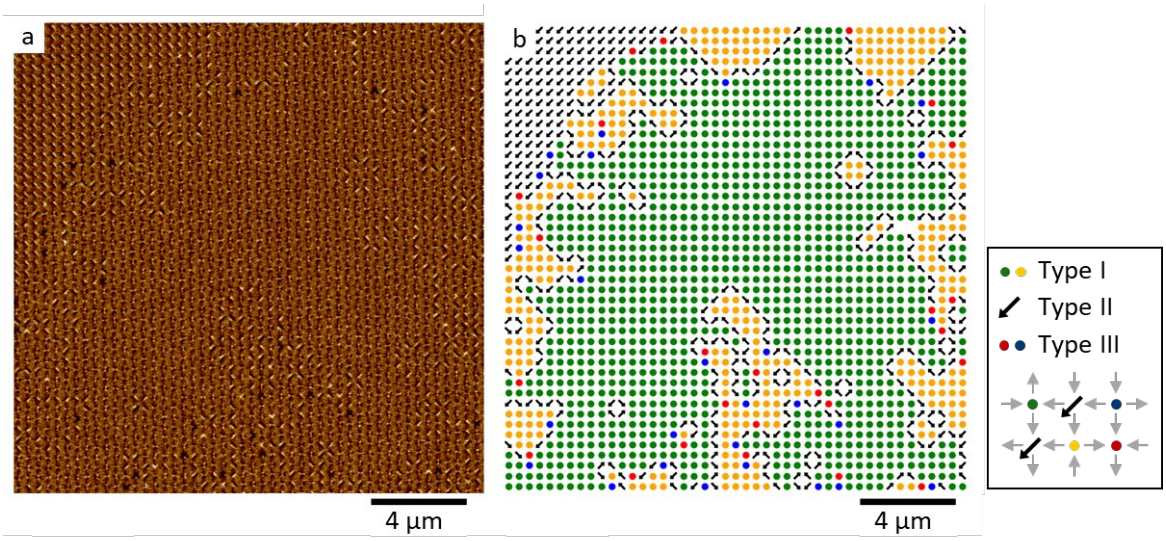


Fig. 1 | (a) Magnetic Force Microscopy (MFM) image of a square artificial spin ice following laser induced magnetic relaxation. (b) The MFM image is converted to colored dots and arrows representing the magnetic configurations at each vertex, which is surrounded by four neighboring nanomagnets. The green and yellow dots indicate the two degenerate Type I vertex configurations associated with the ground state. The two domains are separated by chains of Type II vertex configurations, represented by black arrows pointing in the direction of the net magnetic moment. Finally, a few vertices assume Type III vertex configurations (red and blue dots).

Gantenbein Valentin (non-confidential)

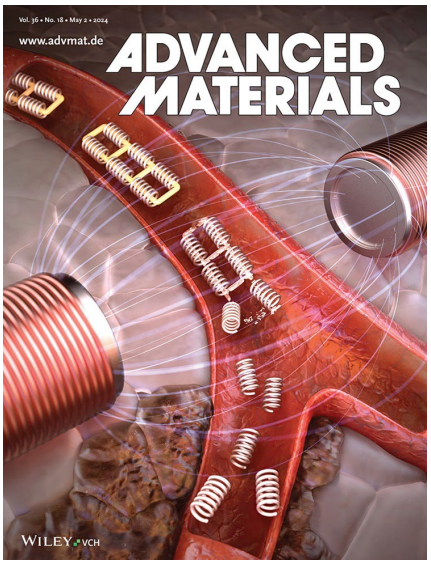
Microrobotic Superstructures for Transport and Delivery of Magnetic Micromachines

Valentin Gantenbein [1], Fabian C. Landers [1], Lukas Hertle [1], Andrea Veciana [1], Joaquin Llacer – Wintle [1], Xiang-Zhong Chen [2], Hao Ye [1], Carlos Franco [1], Josep Puigmartí-Luis [3], Minsoo Kim [1], Bradley J. Nelson [1], Salvador Pané [1]

[1] Multi-Scale Robotics, D-MAVT, ETH Zurich
[2] Fudan University, Institute of Optoelectronics
[3] University of Barcelona, Departament de Ciència dels Materials i Química Física

In the field of biomedical small-scale robotics, the combination of metals and polymers offers opportunities for novel functionalities. Microrobots consisting of metals and organic materials leverage the unique properties of both material classes. Integration of metallic components with polymer structures by combining 3D-Lithography, mold casting and electroplating, yields elevated magnetic responsiveness, increased drug loading capacity, shape adaptability, and elasticity.[1,2] The approach facilitates diverse microrobotic locomotion modes and controlled swarm delivery, demonstrating its versatility across applications.[3] Furthermore, a microrobotic superstructure is introduced comprising interconnected magnetic units organized via a transient physical gelatin chassis. This superstructure, composed of electroplated magnetic helical micromachines interlocked by a gelatin nanocomposite containing iron oxide nanoparticles, exhibits responsive motion and controlled disassembly under various magnetic inputs.[4] Practical demonstrations include swarm navigation in large channels utilizing gradient magnetic fields, disassembly and micromachine release via high-frequency alternating magnetic fields, and corkscrew locomotion of single micromachines through small channels using rotating magnetic fields. This adaptable superstructure holds promise for intricate delivery procedures within the human body, offering a paradigm shift in confined environment navigation.

[1] De Marco et al., Adv. Mater. Technol., 2019
[2] Alcântara et al., Small, 2019
[3] Alcântara et al., Nat. Commun., 2020
[4] Gantenbein et al., Adv. Mater., 2023



The microrobotic superstructure comprises a a magnetic gelatin composite chassis threded with iron helical micromachines. Magnetic inputs can be used to navigate the superstructure and also dissolve the soft polymer chassis through magnetic hyperthermia. The capability of these micromachines to disassemble on-command to access narrower conduits enhances the microrobots' multifunctionality.

Chen Jiuke (non-confidential)

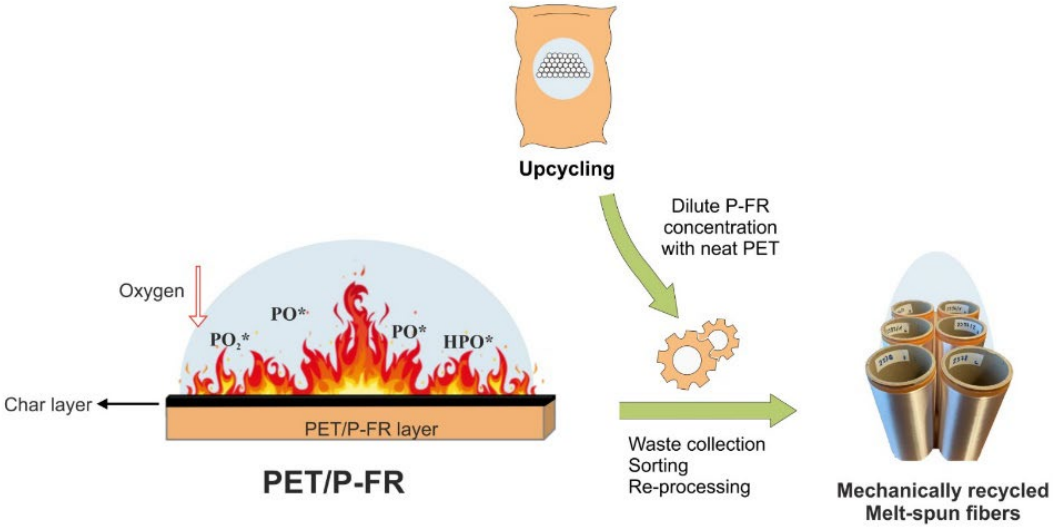
The Role of Phosphorus Flame Retardants in Mechanical Recycling of PET

Jiuke Chen [1-2], Sithiprumnea, Dul [1], Manfred Heuberger [1-2], Rudolf Hufenus [1], Sabyasachi Gaan [1], Ali Gooneie [3]

[1] Advanced Fibers, Empa
[2] D-MATL, ETH Zürich
[3] Circular Plastics, Department of Circular Chemical Engineering, Faculty of Science and Engineering, Maastricht University

To improve the recyclability of polyethylene terephthalate (PET) fabrics containing phosphorus flame retardants (PFRs), the presented study investigates the effects of various FR formulations on the mechanical and fire performance during mechanical recycling. In practical recycling applications, it is a complex task to achieve PET/FR waste free from other FR contamination. Through a combined series of chemical, thermal, and rheological characterizations, we focused on compounds containing a DOPO derivative (DOPO-PEPA, hereinafter referred to as 'DP') and a phosphonate compound (Alfammit PCO 900, hereinafter referred to as 'AF'). We employed time-resolved frequency sweeps (TRFS) to demonstrate that the DP/AF mixture notably stabilizes the melt viscosity of PET over extended processing time even at reduced FR concentration [1], which enables the possibility of pilot-scale repeated processing and melt-spinning trials. After recycling, PET with hybrid DP/AF outperforms PET/AF compounds in terms of mechanical properties and exhibits robust fire performance in fire tests. To further investigate the role of FRs in PET degradation, molecular insights are sought through density functional theory calculations, elucidating the decomposition pathways of FRs, thus paving the way for understanding and improving the recyclability of PET/FR.

[1] J. Chen, et. al., J. Mater. Sci. Technol. 194 (2024) 167–179



Zürcher Dominik (non-confidential)

Real-Time Observation of Protein Aggregation at Liquid-Liquid Interfaces in a Microfluidic Device

Dominik Zürcher [1], Klaus Wuchner [2], Paolo Arosio [1]

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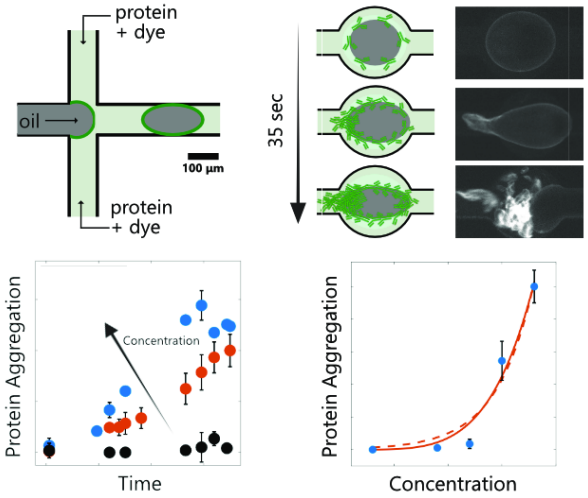
[2] Janssen R&D, DPDS BTDS Analytical Development, Schaffhausen

We describe a droplet microfluidic device to capture in real-time protein aggregation at liquid-liquid interfaces. We simultaneously monitor protein adsorption, the formation of a viscoelastic protein layer, aggregation and shedding of protein particles into solution. We analyze the stability of therapeutic formulations over a wide range of concentrations (1-180 mg/mL) at pharmaceutically relevant liquid interfaces under controlled mechanical deformation. The adsorption onto oil droplets induces the formation of a viscoelastic protein layer on a sub-second timescale, which progressively restricts the relaxation of the droplets within the chip. Upon mechanical rupture, the protein layer releases particles in solution. The rate of particle formation strongly increases with concentration, similarly to bulk viscosity. Concentrations above 120 mg/mL lead to aggregation within seconds and drastically decrease the mechanical perturbations required to shed protein particles in solution. We showcase the power of our approach by a thorough screening of surfactants and excipients to stabilize the protein against interfacial stress. In this context, our low volume microfluidic platform allows to assess protein stability early in development and represents an attractive tool to optimize protein formulations, consuming limited amounts of precious material.

[1] M. R. G. Kopp, F. Grigolato, D. Zürcher et al., J. Pharm. Sci., 112 (2023)



Chen Mary Jialu (non-confidential)

Manufacturing and Characterization of a Novel Composite Heart Valve Prosthesis

Mary Jialu Chen [1], Georgios A. Pappas [1], Caroline C. Smid [1], Nikola Cesarovic [2][3], Volkmar Falk [2][3][4] and Paolo Ermanni [1]

[1] Composite Materials and Adaptive Structures, D-MAVT, ETH Zurich
[2] Translational Cardiovascular Technologies, D-HEST, ETH Zurich
[3] Department for Cardiothoracic and Vascular Surgery, Charité Universitätsmedizin Berlin, Germany
[4] German Center for Cardiovascular Research (DZHK), Partner Site Berlin, Germany

Current cardiovascular implants offer patients an unfortunate compromise between durability and hemocompatibility. By combining polyetheretherketone (PEEK) leaflets with a carbon fiber (CF)/PEEK composite stent, we seek to make heart valves that are both durable and hemocompatible. A melt forming process was used to simultaneously form and attach PEEK leaflets to an autoclave-processed composite stent [1]. This rapid manufacturing process results in a quasi-continuous interface that avoids stress concentrations while allowing for an improved stent-leaflet interface. The forming also results in a controlled annealing which is shown to improve the mechanical performance of processed leaflets through miniaturized tensile and peel testing. Since PEEK is known to be chemically inert in addition to mechanically resilient, hemocompatibility testing was also performed, showing that platelet adhesion decreases with PEEK crystallinity due to altered surface properties [2]. Finally, cyclic testing in a pulse duplicator showed no significant changes in mean pressure differential or regurgitation after 1000 cycles, demonstrating proof of concept. The described manufacturing processes expand the design space of heart valve prostheses and advance the use of composite materials in cardiovascular device technology.

[1] M.J. Chen, et. al., Polymer Composites, *in press* (2024)
[2] M.J. Chen, et. al., Biomaterial Advnaces, 146, 213288 (2023)

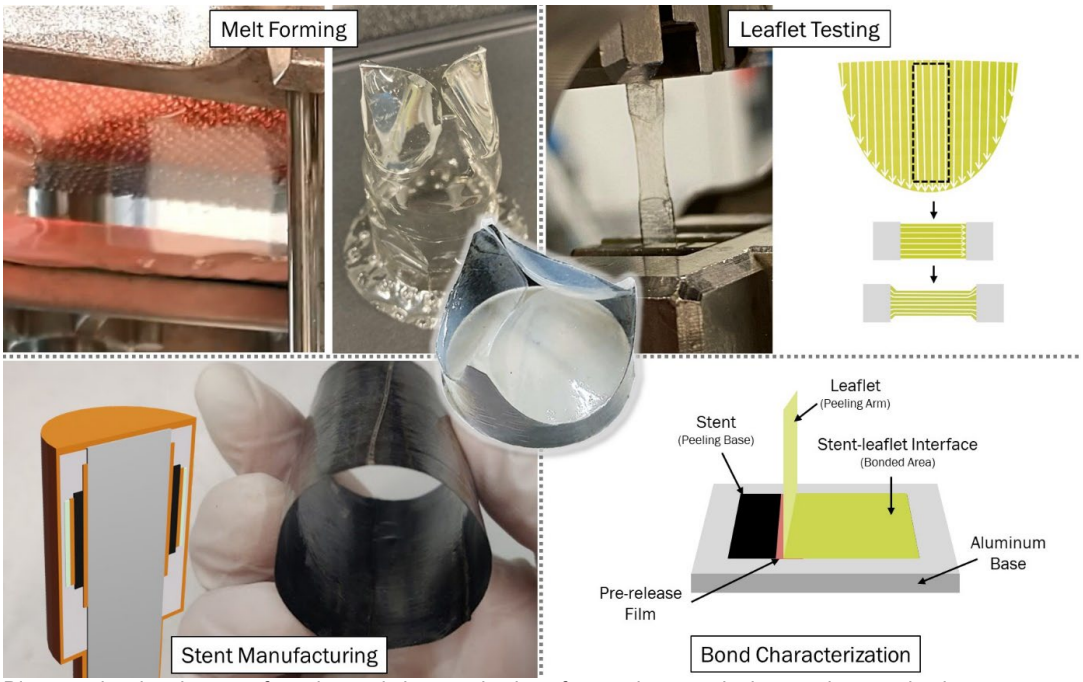


Diagram showing the manufacturing and characterization of a novel composite heart valve prosthesis

Poster Presentations

No.	Name	Poster Title	Dept	Group
1	Agrawal Samarth	Mathematical Methods to Characterize Microstructure of, and Transport in Mesoporous Materials	D-MATL	Computational polymer physics
2	Bang Johee	Noninvasive three-dimensional mapping of local structure in perovskite superlattices	D-MATL	Multifunctional Ferroic Materials
3	Berchialla Luca	Phase Transitions and Magnetic Order in a Ruby Lattice Artificial Spin Ice	D-MATL	Mesoscopic Systems
4	Berlanda Simon	Automated sample management for microfluidic combinatorial antimicrobial susceptibility testing and characterization by microscopy and MALDI-MS	D-BSSE	Bioanalytics Group
5	Bernhard Tim	Reproducing Viscoelastic Behaviours of End-linked Polymer Networks using Simulations	D-MATL	Nanometallurgy
6	Canavan Mark	Imaging the Local Electrochemical Potential of Graphene with Scanning Tunneling Potentiometry	D-MATL	Magnetism and Interface Physics
7	Chen Xiulin	Applications of Bio-based Materials for CO_2 Sequestration in Building Materials	D-BAUG	Durability of Engineering Materials
8	Cheng Hsu-Cheng	Modeling domain evolution in ferroelectric materials	D-MAVT	Mechanics and Materials
9	D'Andria Matteo	Non-equilibrium Synthesis of Metastable Nanocrystals for Molecular Sensing and Catalysis	D-MAVT	Human-centered Sensing Laboratory (HSL)
10	D'Andria Matteo	Structure-Function Relationship of Highly Reactive CuOx Clusters on Co3O4 for Selective Formaldehyde Sensing at Low Temperatures	D-MAVT	Human-centered Sensing Laboratory (HSL)
11	Di Francescantonio Agostino	Electro-Optic Control of Linear and Nonlinear Signals by a Monolithic LiNbO 1D Photonic Crystal	D-PHYS	Optical Nanomaterial (guest PhD Grange Rachel)

No.	Name	Poster Title	Dept	Group
12	Dreimol Christopher	Catalyst Chronicles: Tracing the Structural Evolution and Underlying Mechanisms of Iron-Catalyzed Laser-Induced Graphitization	D-BAUG	Wood Materials Science
13	Du Yinwei	Modeling and Computational Design of Deformable Sheets with Bi-Material Distribution	D-INFK	Computational Robotics Lab
14	Eliasson Henrik	Nanoparticle Size Estimation using Scanning Transmission Electron Microscopy and Generative AI	D-MATL	Multifunctional Materials
22	Enrriquez Casimiro Nadia	Bacteria-driven Precipitation of Calcium Carbonate in Droplets	D-MATL	Complex Materials
15	Feng Yanxia	Freezing Hydrogels Reveals a Simple, Power-law Behavior of their Osmotic Pressure	D-MATL	Soft Materials and Interfaces
16	Giovanoli Diego	Microfluidic Sorting of Biomineralizing Microorganisms	D-MATL	Complex Materials
17	Giulimondi Vera	Evidence of Bifunctionality of Carbons and Single Metal Atoms in Catalyzed Acetylene Hydrochlorination	D-CHAB	Advanced Catalysis Engineering
18	Gómez Cuyàs Judith	Mycooptics. A Multiscale Approach to Understand the Optical Properties of Mycelium	D-MATL	Nanometallurgy
19	Han Zhichao	Unsupervised Learning of Material Behavior in Dynamics	D-BAUG	Computational Mechanics of Building Materials
20	Kaniselvan Manasa	Dynamical Monte Carlo Modelling of Nanoionic Resistive Memory Devices	D-ITET	Computational Nanoelectronics
21	Kazemi Pour Amirhossein	A Synergy of Electrohydraulic Muscles and Electrostatic Clutches for Full Motion Ranges in Musculoskeletal Antagonistic Joints	D-MAVT	Soft Robotics
23	Kindler Robert Oswin	Exploring Living Organisms for Wood-Based Materials	D-BAUG	Wood Materials Science
24	Kiwic David	Nanoparticle Gelation at Tailored pH For Advanced Photocatalysts	D-MATL	Multifunctional Materials

No.	Name	Poster Title	Dept	Group
25	Lohmann Victoria	Chemical Recycling of Poly(methacrylamides): Low Temperature Depolymerization of Biorelevant Polymers	D-MATL	Polymeric Materials
26	Marin Luca	Description of Dark Matter-Electron Scattering in Liquid Xenon Targets via Density Functional Theory	D-MATL	Materials Theory
27	Medany Mahmoud	Ultrasound Microrobots Navigate Against the Flow Using Model-Based Reinforcement Learning	D-MAVT	Acoustic Robotics system lab (ARSL)
28	Mlkvik Peter	Metal-insulator Transition in VO_2 within a Bond-centered Approach	D-MATL	Materials Theory
29	Pereira Martins Michael	Template-free and dry synthesis of highly porous metal nitride architectures for electronics and molecular sensing	D-MAVT	Human-centered Sensing
30	Porenta Nikolaus	Composition Control of Alloy Fabrication Using Localized Electrochemical Deposition for Small-Scale Additive Manufacturing	D-MATL	Nanometallurgy
31	Pozzi Marcello	Symmetry breaking in plasmonic meta-atoms based on quantum graphs	D-MATL	Nanometallurgy
32	Prountzou Eleni	Fabrication and Characterization of Polycrystalline Barium Titanate Films for Integrated Quantum Devices	D-PHYS	Optical Nanomaterial Group
33	Reiter Manuel	Controlled Halogenation of the Solid Electrolyte Interphase in Li Metal Batteries	D-MAVT	Electrochemical Energy Systems
34	Rich Andrea	*In vivo* sensors to characterize Mg and Ti implants	D-MATL	Metal Physics and Technology
35	Schenk Florian	Phase-change memory from molecular tellurides	D-ITET	Chemistry and Materials Design
37	Scherrer Simon	Characterising Rough and Adhesive Single-Particle Contacts	D-MATL	Laboratory for Soft Materials and Interfaces
38	Seda David	Nanoimprint Lithography of Optical Fourier Surfaces	D-MAVT	Optical Materials Engineering
39	Sifringer, Léo	Interfacing Soft Electronics and Engineered Neuronal Networks: a Nerve-on-a-Chip Model Towards Biohybrid Electronics	D-ITET	Biosensors and Bioelectronics

No.	Name	Poster Title	Dept	Group
40	Simmen Edith	Interplay of metallicity, ferroelectricity and layer charges: A DFT study of $SmNiO_3$ and $BaTiO_3$ superlattices	D-MATL	Materials Theory
41	Smid Caroline	Buckling-Inspired Heart Valve Leaflet Designs for Stiff Polymeric Materials	D-MAVT	Composite Materials and Adaptive Structures
42	Song Chao	Droplet-based Fabrication of Soft Microrobots with Tailored Magnetic Anisotropy	D-CHAB	Microfluidics
43	Stanko Štefan T.	Structural and Thermal Characterization of Zr-Based Bulk Metallic Glasses via Fast Differential Scanning Calorimetry and Synchrotron X-Ray Diffraction	D-MATL	Metal Physics and Technology
44	Veciana Andrea	Breaking the PFAS Chain: Piezocatalytic Decomposition of Forever Chemicals Using $BaTiO_3$ Nanoparticles	D-MAVT	Multi-Scale Robotics
45	Wang Hanchen	Understanding the magnetic properties of ultrathin BiYIG grown by sputtering	D-MATL	Magnetism and Interface Physics
46	Winters Arturo	Pioneering Fluctuations in Viscoelastic Stress: A Comparison of the Temporary Network and Dumbbell models	D-MATL	Soft Materials
47	Wintersteller Simon	Unravelling the Amorphous Structure and Crystallization Mechanism of GeTe Phase Change Memory Materials	D-ITET	Chemistry and Materials Design
48	Wolfisberg Gianna (& Bittmann Pablo Camilo)	Impact of Induced Spontaneous Curvature on the Shape of Adhered, Phase Separated Pancake-like GUV's and Their Digital Reconstruction as a Mesh	D-MATL	Soft Materials
49	Xie Chang	High-efficient Engineering of Osteo-callus Organoids for Rapid Bone Regeneration Within One Month	D-HEST	Biomaterials Engineering

Abstracts of Posters

1 **Agrawal Samarth** (non-confidential)

Mathematical Methods to Characterize Microstructure of, and Transport in Mesoporous Materials

Samarth Agrawal [1] [2], Sandra Galmarini [2], and Martin Kröger [2]

[*1] Computational polymer physics, D-MATL, ETH Zurich*
[2] Advanced colloidal materials engineering, Building energy and materials, Empa

We develop and implement mathematical methods to characterize the microstructure and transport properties of mesoporous materials, with a specific focus on silica aerogels. Our methods introduce the concept of critical bonds [1], which are essential for characterizing contact-based transport within these materials. Additionally, we rigorously define the geometric pore-size distribution (PSD) [2] and introduce a new, highly efficient algorithm based on Voronoi tessellation to calculate the PSD [3].

Using diffusion-limited aggregation algorithms, we create model structures that mimic the microstructure of silica aerogels [4]. These theoretical models are then validated against experimental data, including Small-Angle X-ray Scattering (SAXS) measurements, density analysis, and PSD results. The comparison between our theoretical predictions and experimental observations demonstrates the accuracy and robustness of our methods.

Furthermore, we investigate the transport properties within these model structures by simulating the Fokker-Planck equation.[5] This allows us to gain insights into the mechanisms underlying Knudsen pumps, which are critical for understanding gas transport in mesoporous materials. Our simulation results provide a detailed understanding of how the microstructural characteristics influence transport phenomena, highlighting the importance of pore connectivity and size distribution.

Overall, our research contributes to a comprehensive framework for analyzing and predicting the behavior of mesoporous materials. The methods and insights developed in this study have potential applications in various fields, including material science, chemical engineering, and nanotechnology. By bridging the gap between theoretical modeling and experimental validation, we pave the way for the design and optimization of advanced materials with tailored transport properties.

[1] Agrawal et al., *Phys. Rev. Lett.,* 132 (19), 196101
[2] Agrawal et al., *Phys. Rev. E,* 107 (1), 015307
[3] Kröger et al., *Comp. Phys. Comm.,* 301, 109212
[4] Hasmy et al., *Phys. Rev. B,* 50, 6006
[5] Agrawal et al., *J. Fluid. Mech.,* 899 A25

2 **Bang Johee** (non-confidential)

Noninvasive three-dimensional mapping of local structure in perovskite superlattices

J. Bang [1], N. Strkalj [2], M. Trassin [1], T. Weber [1]

[1] Multifunctional Ferroic Materials, D-MATL, ETH Zurich
[2] Institute of Physics, Zagreb

In functional oxide thin film research, understanding the origin of the order parameter and learning how to manipulate it has always been one of the core objectives. The materials often display delicate interaction among spin, orbital, and lattice order parameters, and with the development of thin film deposition technique, we can even introduce various emergent phenomena by artificially engineering heterointerfaces and superlattices of oxide layers. One example is the superlattices of short-period ferroelectric lead titanate and dielectric strontium titanate, which have ordered arrays of polar-skyrmion bubbles [1]. So far, structural investigation of the skyrmion domains was mainly achieved through destructive analysis or spatially limited classical structural analysis. Noninvasive investigation of the domains in large three-dimensional volume remains elusive, which holds promise for understanding the structure and distribution of the domains in detail. Here, we report on non-invasive three-dimensional mapping of local structure via a large volume reciprocal space investigation. Specifically, we collected a comprehensive three-dimensional diffuse scattering data using synchrotron hard X-rays at ultra-small grazing-incidence geometry. The data was analyzed with three-dimensional delta pair distribution function (3D-ΔPDF) method [2], which allowed us to acquire information about the three-dimensional distribution of the skyrmion domains. This experimental approach opens door for real structure investigation of thin films as such information is not readily accessible with common characterization techniques such as Piezoresponse Force Microscopy (PFM) or Transmission Electron Microscopy (TEM).

[1] S. Das et al., *Nature* 568, 368-372 (2019)
[2] T. Weber & A. Simonov, *Z. Kristallogr.* 227, 238-247 (2012)

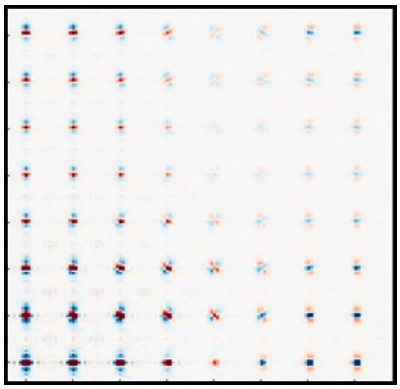


Figure 1. 3D-ΔPDF of the extracted diffuse rings from the collected three-dimensional reciprocal space, which are the signatures of skyrmion domains.

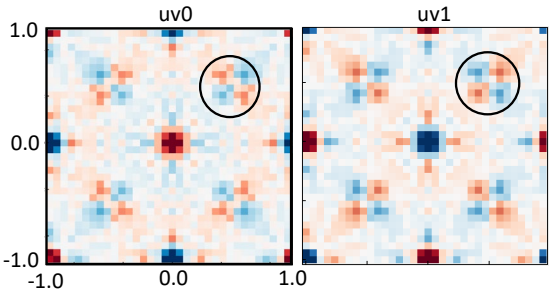


Figure 2. 3D-ΔPDF of extracted half-integer streaks from the collected three-dimensional reciprocal space, which are the signatures of octahedral tilts.

3 **Berchialla Luca CONFIDENTIAL**

Phase Transitions and Magnetic Order in a Ruby Lattice Artificial Spin Ice

Luca Berchialla [1,2], Gavin M. Macauley [1,2],Tianyue Wang [1,2], Anja Weber [1,2], Armin Kleibert [3], Valerio Scagnoli [1,2], Peter M. Derlet [1,4], Laura J. Heyderman [1,2].

[1] Mesoscopic Systems, D-MATL, ETH Zurich
[2] Multicale Materials Experiments, PSI
[3] Swiss Light Source, PSI
[4] Condensed Matter Theory, PSI

4 **Berlanda Simon F.** (non-confidential)

Automated sample management for microfluidic combinatorial antimicrobial susceptibility testing and characterization by microscopy and MALDI-MS

Simon F. Berlanda [1], Maximilian Breitfeld [1], Robert Strutt [1] and Petra S. Dittrich[1]

[1] Bioanalytics, D-BSSE, ETH Zurich

The surge in antibiotic resistance poses a severe threat to global health, rendering former efficacious drugs ineffective against bacterial infections. Projections forecast a substantial toll in mortality, with additional considerations for opportunistic infections arising from co-morbidities. Conventional approaches to screening novel antibiotics and profiling patient samples for therapeutic guidance often entail laborious and resource-intensive procedures characterized by limited throughput. Consequently, innovative screening platforms capable of rapid and cost-effective testing are urgently needed.

Through adaptations to our proprietary droplet spotting platform, we are capable of generating massive open droplet arrays comprising individual sample droplets within the nanoliter scale. We deposit thousands of droplets on the surface of a glass plate, while preventing evaporation by use of an oil cover. Using this platform, we encapsulate bacterial specimens and expose them to different antibiotics at various concentrations and in various combinations. Subsequent observation via time-lapse microscopy unveils the cell responses, either continuous growth for resistant cells, stopped growth in case of persistant cells, or cell death and lysis in case of susceptible cells.

A great benefit of this novel platform is its versatility with respect to the analytical methods for monitoring the bacterial cells. Beyond routinely used microscopy, the integration of MALDI-mass spectrometry enables rapid profiling of biomolecules, thereby could facilitate the discovery of resistance biomarkers in future work.

[1] U. Theuretzbacher, et al., Nat. Rev. Microbiol., 18:286-298 (2020)
[2] S. Needs, et al., Front. Mech. Eng., Vol6 (2020)
[3] P. Jusková, et al., ACS Sens., 6:2202–2210 (2021)
[4] D. Haidas, et al., 91:2066-2073 (2019)

5 **Bernhard Tim** (non-confidential)

Reproducing Viscoelastic Behaviours of End-linked Polymer Networks using Simulations

Tim Bernhard, Prof. Dr. Andrei Gusev

[1] Nanometallurgie, D-MATL, ETH Zurich

Molecular simulations of polymer networks allow for otherwise impossible insights into the relationship between the microscopic structure and the macroscopic properties of materials. Current simulation studies are limited to relatively small systems and/or short time scale, making accurate predictions of macroscopic viscoelastic properties difficult. This is especially true for highly fluctuating systems such as damping elastomers or near-critical polymer networks (networks that just passed the solution-gel transition). Understanding the influence of the microscopic structure on the macroscopic properties would be of special interest for such network systems, as they could serve important applications for example in medicine and health technology. Here we assess the current possibilities, limitations and computational requirement needed to reproduce experimental data of storage and loss moduli of such end-linked network systems using classical Kremer-Grest Molecular Dynamics simulations and Dissipative Particle Dynamics simulations with slip-springs.

6 **Canavan Mark** (non-confidential)

Imaging the Local Electrochemical Potential of Graphene with Scanning Tunneling Potentiometry

Toni Marković [1], Wei Huang [1], Mark Canavan [1], Jeong Ah Seo [1], Pietro Gambardella [1], and Sebastian Stepanow [1]

[1] Magnetism and Interface Physics, D-MATL, ETH Zurich

Two-dimensional material systems and heterostructures have recently emerged as a promising class of materials for high performance electronic devices. In such systems, understanding the influence nanoscale transport effects, such as scattering at atomic defects and interfaces is crucial. Scanning Tunneling Potentiometry (STP) allows for studying charge transport on the nanoscale by relating the local electro-chemical potential to morphological features of the system. STP maintains the angstrom spatial sensitivity of conventional STM while imaging mod- ifications to the ECP with uV resolution, offering a way to potentially investigate transport phenomena beyond the diffusive regime. Here, we present an implementation of STP in a commercial RHK Pan-Scan STM with an integrated flow cryostat capable of reaching tempera- tures of 12K [1]. We perform STP on epitaxial graphene to measure the sheet resistance of monolayer and bilayer grown on SiC as well resistances of interfaces between them. To investigate transport effects beyond the diffusive regime, using back-gated graphene samples would allow for STP measurements with charge carries at the Dirac point.

[1] T. Marković et al. Rev. Sci. Instrum. 92, 103707 (2021)

7 **Chen Xiulin** CONFIDENTIAL

Applications of Bio-based Materials for CO_2 Sequestration in Building Materials

Xiulin Chen [1], Yuqing Dai [1], Dr. Zhidong Zhang [1], and Prof. Ueli Angst [1]

[1] Durability of Engineering Materials, D-BAUG, ETH Zurich

8 **Cheng Hsu-Cheng** (non-confidential)

Modeling domain evolution in ferroelectric materials

Hsu-Cheng Cheng [1], Roman Indergand [1], Khiem Nguyen [2], Laurent Guin [3], and Dennis M. Kochmann [1]

[1] Mechanics & Materials, D-MAVT, ETH Zurich
[2] University of Glasgow
[3] École Polytechnique

The present study employs both computational and analytical approaches to investigate the influence of domain evolution on polarization switching in ferroelectric materials. Phase-field models represent a prevalent computational interface tracking technique employed in the modeling of domain evolution on the mesoscale. Despite the simplicity offered by Allen-Cahn type phase-field models, they are unable to incorporate nonlinear kinetic relation, which are relations between the thermodynamics driving force and the domain wall velocity, of the material [1-3]. To address this limitation, we developed a general kinetic phase-field model that can successfully evolve the domain wall in accordance with the prescribed kinetic relation. During the study of phase-field models, it became evident that there is a paucity of knowledge regarding the influence of material parameters and applied loadings on domain evolution. To this end, we adopted the analytical sharp-interface description of the domain wall to study the influence of permittivity, elasticity, and piezoelectricity on the driving force on a ferroelectric nucleus. Our findings indicate that anisotropic material properties play a pivotal role in nucleus growth. Furthermore, a comparison of the driving forces from the two models revealed that the phase-field model exhibited an additional numerical interfacial energy contribution, which is often negligible in a real material on the mesoscale. Although this numerical interfacial energy is undesirable, it is a characteristic of the model because of the diffuse interface description of the domain wall. To reduce this interfacial energy, we investigate another interface tracking technique: level-set methods [4]. Our preliminary finding showed that the nucleus evolves in a near interfacial-energy-free manner when using this mode

[1] Chen, Long-Qing., *Annual review of materials research* 32.1 (2002): 113-140.
[2] Indergand, Roman, et al., *Journal of the Mechanics and Physics of Solids* 144 (2020): 104098.
[3] Guin, Laurent, and Dennis M. Kochmann., *Journal of the Mechanics and Physics of Solids* 176 (2023): 105301.
[4] Osher, Stanley, and James A. Sethian., *Journal of computational physics* 79.1 (1988): 12-49.

9 **D'Andria Matteo** CONFIDENTIAL

Non-equilibrium Synthesis of Metastable Nanocrystals for Molecular Sensing and Catalysis

Matteo D'Andria [1], Tiago Elias Abi-Ramia Silva [1], Edoardo Consogno [1], Frank Krumeich [2], and Andreas T. Güntner [1]

[1] Human-centered Sensing, D-MAVT, ETH Zurich
[2] Inorganic Chemistry, D-CHAB, ETH Zurich

10 **D'Andria Matteo** (non-confidential)

Structure-Function Relationship of Highly Reactive CuO_x Clusters on Co_3O_4 for Selective Formaldehyde Sensing at Low Temperatures

Matteo D'Andria [1], Frank Krumeich [2], Zhangyi Yao [3], Feng Ryan Wang [3], and Andreas T. Güntner [1]

[1] Human-centered Sensing, D-MAVT, ETH Zurich,
[2] Inorganic Chemistry, D-CHAB, ETH Zurich
[3] Department of Chemical Engineering, University College London, United Kingdom

Designing reactive surface clusters at the nanoscale on metal-oxide supports enables selective molecular interactions in low-temperature catalysis and chemical sensing. Yet, finding effective material combinations and identifying the reactive site remains challenging and an obstacle for rational catalyst/sensor design. Here [1], the low-temperature oxidation of formaldehyde with CuO_x clusters on Co_3O_4 nanoparticles is demonstrated yielding an excellent sensor for this critical air pollutant. When fabricated by flame-aerosol technology, such CuO_x clusters are finely dispersed, while some Cu ions are incorporated into the Co_3O_4 lattice enhancing thermal stability. Infrared spectroscopy of adsorbed CO (Figure 1a), X-ray absorption spectroscopy (Figure 1b) and temperature-programmed reduction in H_2 (Figure 1c) identified Cu^+ and Cu^{2+} in these clusters as active sites. Remarkably, the Cu^+ surface concentration correlated with the apparent activation energy of formaldehyde oxidation (Spearman's $\rho = 0.89$) and sensor response (0.96, Figure 1d), rendering it a performance descriptor. At optimal composition, such sensors detected even the lowest formaldehyde levels of 3 parts-per-billion (ppb) at 75°C (Figure 1e).

[1] M. D'Andria, et al., Adv. Sci. 11, 2308224 (2024)

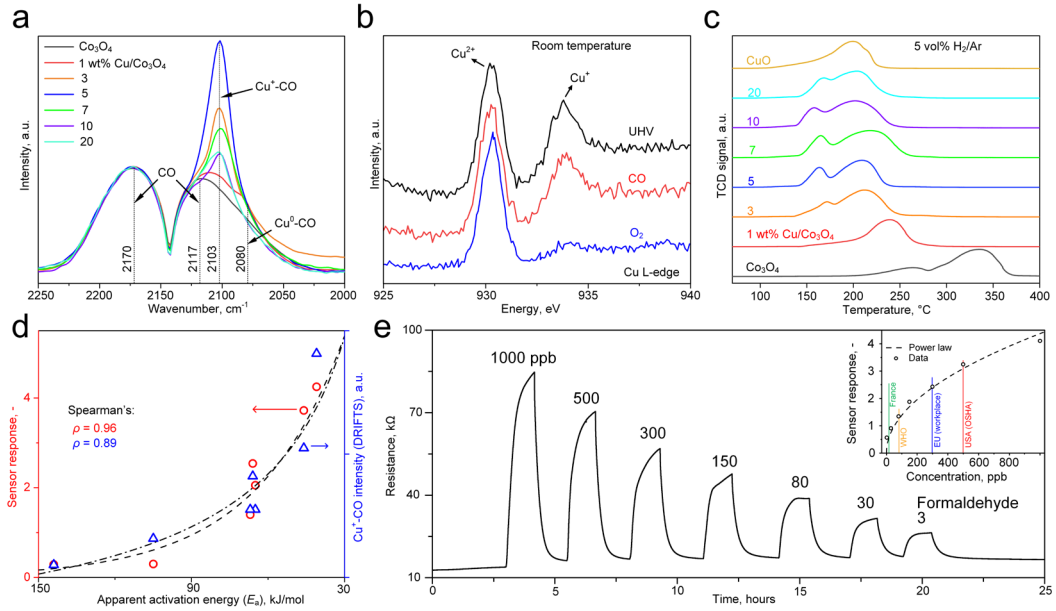


Figure 1: (a) IR spectroscopy of CO adsorbed on 0 – 20 wt% Cu/Co_3O_4 powders with indicated stretches associated with carbonyl group in the gas phase, as well as interacting with surface Cu^+ and Cu^0 species. (b) Near-edge X-ray absorption spectroscopy at the Cu L_3 edge of 5 wt% Cu/Co_3O_4, recorded in Auger electron yield, under ultra-high vacuum (UHV), CO and O_2 at 298 K. Indicated are the peaks associated with the presence of Cu^{2+} and Cu^+ at approximately 930 and 934 eV, respectively. (c) Temperature-programmed reduction profiles of such Cu/Co_3O_4 powders under 5 vol% H_2/Ar between 75 – 400 °C. (d) Scatter plot of sensor response (left ordinate) and IR intensity of Cu^+-CO vibration (right ordinate) over the apparent activation energy (E_a) for formaldehyde oxidation. Spearman's coefficient (ρ) are indicated. Note that the dashed line and dash-dotted line represent the best fit to relate E_a to sensor response and IR intensity, respectively. (e) Ohmic resistance of a 5 wt% Cu/Co_3O_4 film under exposure to 1000, 500, 300, 150, 80, 30, and 3 ppb of formaldehyde in air at 50% RH and 75 °C. Inset shows the corresponding responses with indicated exposure limits in the USA, EU, FR and the WHO guideline.

11 **Di Francescantonio Agostino** (non-confidential)

Electro-Optic Control of Linear and Nonlinear Signals by a Monolithic LiNbO 1D Photonic Crystal

Agostino Di Francescantonio [2], Alessandra Sabatti [1], Maria Antonietta Vincenti [3], Elise Bailly [1], Helena Weigand [1], Luca Carletti [3], Attilio Zilli [2], Marco Finazzi [2], Michele Celebrano [2] and Rachel Grange [1]

[1] Optical Nanomaterials, D-PHYS, ETH Zurich
[2] Politecnico di Milano, Physics Department, Milano, Italy
[3] Università degli Studi di Brescia, Brescia, Italy

Performing free-space optical signals control by means of electro-optic modulation with metasurfaces remains an extremely challenging task to date due to the perturbative nature of the nonlinear interaction underpinning such effect [1]. This is even more true to control upconverted optical signal, which however could produce much stronger modulations thanks to the absence of background. To effectively tackle this problem, we propose a scheme based on a onedimensional, top-down lithium-niobate (LN) photonic crystal hosting high quality factor spectral features in the communication band (Cband) associated with quasi bound states in the continuum (qBIC) [2]. qBIC are beneficial, specifically to the Pockels effect, since a small modification of the refractive index can produce a sizeable change in the signal due to the resonance shift. We reached a modulation in the reflection of a CW laser up to 10% employing CMOS compatible driving voltage (~10V), with bandwidth reaching at least 600 MHz. Moreover, we were able to attain sizeable second-harmonic generation (SHG) by the CW laser using relatively low pump intensities (2.5 kW/cm^2) by matching its wavelength with that of the qBIC. SHG on the enhanced 10 times with respect to the bare LN film. By taking advantage of the quadratic dependence of the SHG on the fundamental field, we demonstrate static electro-optic tuning of the SHG intensity above 70%. In conclusion, we realized an optimized LN platform for CMOS-compatible electro-optic modulation, capable of working both in linear and, for the first time to the best of our knowledge, in the nonlinear regime.

[1] E. Weigand, et. al., ACS Photonics, 8, 3004-3009 (2021) [2] L. Huang, et al., Nat. Commun. 14, 3433 (2023)

12 **Dreimol Christopher** **CONFIDENTIAL**

Catalyst Chronicles: Tracing the Structural Evolution and Underlying Mechanisms of Iron-Catalyzed Laser-Induced Graphitization

Christopher H. Dreimol [1,2], Ronny Kürsteiner [1,2], Maximilian Ritter [1,2], Annapaola Parrilli [3], Jesper Edberg[4], Jonas Garemark[1], Sandro Stucki[1,2], Wenqing Yan, Guido Panzarasa [1],Ingo Burgert [1,2]

[1] Wood Materials Science, D-BAUG, ETH Zurich
[2] WoodTec group, Cellulose and Wood Materials, Empa
[3] Center for X-ray Analytics, Empa
[4] RISE Research Institutes of Sweden, Digital Systems, Smart Hardware, Bio- and Organic Electronics, Norrköping, Sweden

13 **Du Yinwei** (non-confidential)

Modeling and Computational Design of Deformable Sheets with Bi-Material Distribution

Juan Montes Maestre [1], Yinwei Du [1], Ronan Hinchet [2], Stelian Coros [1], Bernhard Thomaszewski [1]

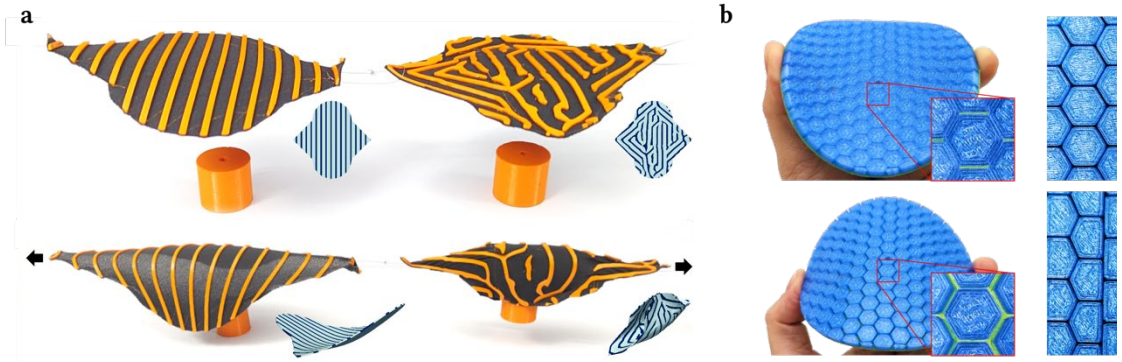
[1] Computational Robotics, D-INFK, ETH Zurich
[2] Soft Robotics, D-MAVT, ETH Zurich

We introduce differentiable stripe patterns and flexible scaled sheets, two families of deformable sheets with bi-material distribution.

In the first work, we propose a computational approach for automated design of stripe-shaped structural surfaces. Our method builds on the work by Knöppel [1] for generating globally-continuous and equally-spaced stripe patterns. We propose a gradient-based optimization tool to automatically compute stripe patterns that best approximate macromechanical performance goals. Specifically, we propose a computational model that combines solid shell finite elements with XFEM for accurate and fully-differentiable modeling of elastic bi-material surfaces. We combine these components with equilibrium state derivatives into an end-to-end differentiable pipeline that enables inverse design of mechanical stripe patterns.

In the second work, we present FlexScale, 3D-printed hard scales are embedded in a soft substrate. we propose a contact-aware homogenization approach that distils native-level simulation data into a novel macromechanical model. This macro-model combines piecewise-quadratic uniaxial fits with polar interpolation using circular harmonics, allowing for efficient simulation of large-scale patterns. We apply our approach to explore the space of isohedral scale patterns, revealing a diverse range of anisotropic and nonlinear material behaviors.

[1] Knöppel, F., et.al., (2015). Stripe patterns on surfaces. ACM Transactions on Graphics (TOG), 34(4), 1-11.



Optimization of a compliant gripper using Differentiable Stripe Patterns
Flexible scaled sheets with different mechanical behaviors for different bending directions and patterns

14 **Eliasson Henrik** (non-confidential)

Nanoparticle Size Estimation using Scanning Transmission Electron Microscopy and Generative AI

Henrik Eliasson [1], Angus Lothian [2], Rolf Erni [1]

[1] Electron Microscopy Center, Empa
[2] Computer Vision Laboratory, Linköping University

One of the most common applications of transmission electron microscopy within nanoparticle catalysis is the assessment of particle size distribution in samples. This assessment often relies on quantifying particle sizes by diameter, a simplification necessitated by the lack of effective techniques for bridging the gap between experimental images and atomic models. In this work, we investigate the use of generative adversarial networks (GANs) to overcome this limitation. We present a substantial dataset of simulated physical images of Pt particles on ceria, alongside a comprehensive experimental dataset obtained through high-resolution scanning transmission electron microscopy of the same system. We successfully teach a cycle-consistent generative adversarial network to map between these two image domains, and train a size-estimation network to output the number of atoms of an imaged nanoparticle. Applying our size-estimator to over 100 imaged particles from a Pt/CeO2 catalyst yields a realistic size distribution with a mean particle size of 137 atoms.

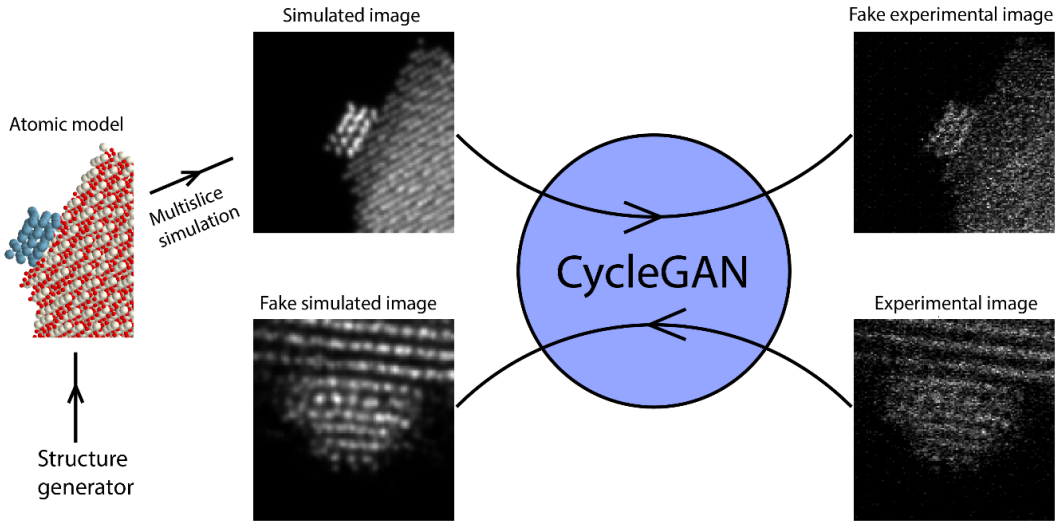


Figure 1: Our cycleGAN effectively carries out the style transfer task, mapping simulated images to what they would look like if the structure was imaged in the microscope. Conversely, sending real experimental images through the cycleGAN is like applying a potent denoising algorithm.

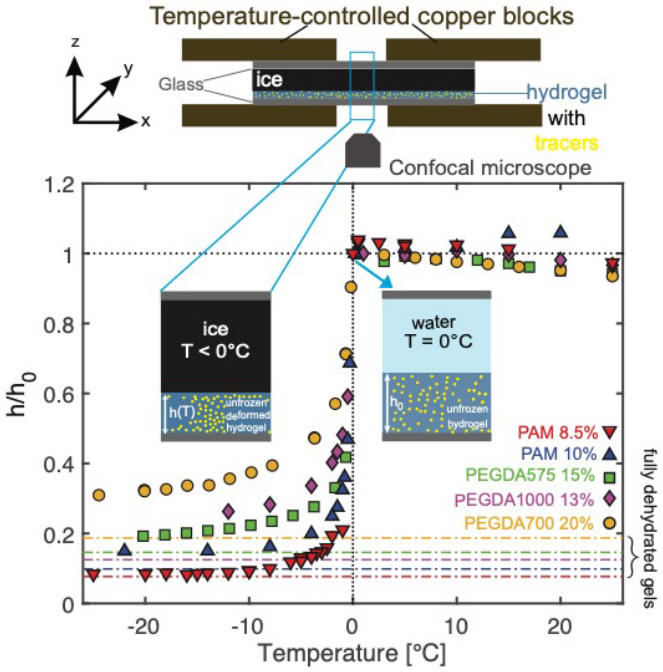
15 **Feng Yanxia** (non-confidential)

Freezing Hydrogels Reveals a Simple, Power-law Behavior of their Osmotic Pressure

Yanxia Feng [1], Dominic Gerber [1], Stefanie Heyden[2], Martin Kröger [3], Eric Dufresne [4], Lucio Isa [1] and Robert Style [1]

[1] Soft Materials and Interfaces, D-MATL, ETH Zurich
[2] Computational Mechanics, D-BAUG, ETH Zurich
[3] Computational Polymer Physics, D-MATL, ETH Zurich
[4] Soft and Living Materials, Department of Materials Science and Engineering, Cornell University

Hydrogels are particularly versatile materials that are found across a wide range of natural and industrial applications. One key reason for this versatility is their high water content, which lets them dramatically change their volume and many of their material properties – often by orders of magnitude – as they swell and dry out. To understand hydrogel behavior, we need techniques to characterize how these properties change across a range of different water contents. Here, we show that one approach is to use Gel-Freezing Osmometry (GelFrO), an extension of freezing-point osmometry(FPO), which is commonly used to characterize aqueous solutions. We re-imagine FPO to apply to hydrogels by tracking the shrinkage of a gel layer in contact with ice. We demonstrate GelFrO for several different hydrogels, by measuring their mechanical response to compression and their osmotic pressure as a function of polymer content. We use the results to derive a new, broadly applicable constitutive model for hydrogel mechanical behavior. Moreover, we compare the results with classical gel-swelling theoretical predictions, and do not find good agreement. Instead our data is well-described by simple power-law expressions. We interpret this as a hallmark of a microscopic fractal structure of the gel's polymer network, and propose a simple way to connect the gel's fractal dimension to its mechanical properties. GelFrO offers many advantages over current approaches, including the ability to work with small samples, the need for only relatively short equilibration times, and the fact that it gives access to a wide range of gel compressions. This technique helps us understand mechanical and osmotic pressure behaviour of hydrogels.



The equilibrium thickness of hydrogel layers in contact with bulk ice/water. Top: schematic of the freezing stage. Bottom: change in hydrogel layer thickness as a function of temperature – relative to the thickness at T = 0°C. Above 0°C, hydrogels are in equilibrium with bulk water, and there is only a small dependence of film thickness on

temperature. Below 0°C, hydrogels are in contact with bulk ice, and shrink with increasing undercooling. Shrinkage is caused by cryosuction from the ice drawing water out of the hydrogel. Dash dotted lines show the thickness of fully-dehydrated gels – i.e. dry polymer.

16 Giovanoli Diego CONFIDENTIAL

Microfluidic Sorting of Biomineralizing Microorganisms

Diego Giovanoli [1], Dr. Anton Kan [1], and Prof. André Studart [1]

[1] Complex Materials, D-MATL, ETH Zurich

17 **Giulimondi Vera** (non-confidential)

Evidence of Bifunctionality of Carbons and Single Metal Atoms in Catalyzed Acetylene Hydrochlorination

[1] Advanced Catalysis Engineering, D-CHAB, ETH Zurich
[2] ICIQ-CERCA
[3] Photon Science Division, PSI

Carbon supports are ubiquitous in heterogeneous catalysts for acetylene hydrochlorination to vinyl chloride, from commercial Hg-based systems to sustainable metal single-atom alternatives. Their potential co-catalytic role has been postulated but not unequivocally demonstrated. Here, we evidence the bifunctionality of carbons and single metal atoms (Pt, Au, Ru) in catalyzing acetylene hydrochlorination by using a multi-technique approach to monitor their structure from synthesis to operation. Operando X-ray absorption spectroscopy shows that metal atoms from various synthesis methods have similar dynamic behaviors but different catalytic performances, with metal atoms exclusively activating HCl (Figure 1a). In contrast, modifications to the carbon matrix during synthesis are crucial, revealing the co-catalytic role of metal-neighboring sites in binding C2H2, as determined by spectroscopy, sorption, and kinetic analyses (Figure 1b). This bifunctional behavior is observed across different metals and carbons, suggesting a general mechanism. Resolving the coordination environment of working metal atoms guides theoretical simulations in rationalizing C2H2 adsorption on metal-neighboring carbon functionalities (Figure 1c). Finally, coking of the latter ones (Figure 1d) is identified as the leading deactivation pathway.

[1] P. Johnston, et al., J. Am. Chem. Soc. 137, 14548 (2015)
[2] V. Giulimondi, et al., Nat. Commun. 14, 5557 (2023)

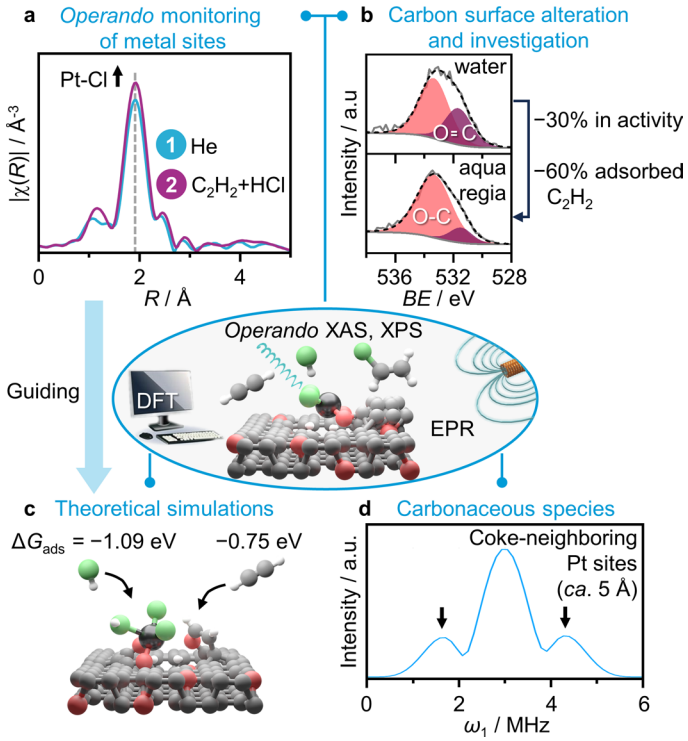


Figure 1. Schematic of the multi-technique approach employed. (a) *Operando* Pt L_3 edge extended X-ray absorption fine structure. (b) O 1*s* X-ray photoelectron spectra of the carbon functionalities following synthesis procedures employing distinct solvents. (c) Density functional theory simulations encompassing metal and neighboring carbon sites. (d) Electron paramagnetic resonance analysis of coke deposits.

18 **Gómez Cuyàs Judith** (non-confidential)

Mycooptics. A Multiscale Approach to Understand the Optical Properties of Mycelium

Judith Gómez Cuyàs [1], Moritz Garger [1], Blanka Oliwia Sokolowska [2], Markus Künzler [2], Henning Galinski [1] and Ralph Spolenak [1]

[1] Nanometallurgy, D-MATL, ETH Zurich
[2] Microbiology, D-BIOL, ETH Zurich

Mycelium, the root-like structure of fungi, offers a largely unexplored area in the field of optics. Due to its intricate hierarchical and anisotropic properties, mycelium constitutes a complex optical medium that poses significant challenges for understanding and controlling transport dynamics. This research aims to investigate and manipulate the relationship between the hierarchical structure of fungal networks and its properties, to harness their potential for light manipulation. We propose the functionalization of the organism's growth as a strategy to engineer its optical characteristics. Key questions addressed in this work include: How does mycelium interact with light? How is light transported through mycelial networks? What constituents participate in the optical response of the system? Can we use mycelial networks to manipulate light? Through this research, we seek to develop a foundational understanding that could pave the way for innovative applications of mycelium in optical applications.

19 **Han Zhichao CONFIDENTIAL**

Unsupervised Learning of Material Behavior in Dynamics

Zhichao Han [1], Mohit Pundir [1], Olga Fink [2], and David S. Kammer [1]

[1] Computational Mechanics of Building Materials, D-BAUG, ETH Zurich
[2] Intelligent Maintenance and Operations Systems, ENAC, EPFL

20 **Kaniselvan Manasa CONFIDENTIAL**

Dynamical Monte Carlo Modelling of Nanoionic Resistive Memory Devices

Manasa Kaniselvan [1], Marko Mladenovic [1], Alexander Maeder, and Mathieu Luisier [1]

[1] Computational Nanoelectronics, D-ITET, ETH Zurich

21 **Kazemi Pour Amirhossein CONFIDENTIAL**

A Synergy of Electrohydraulic Muscles and Electrostatic Clutches for Full Motion Ranges in Musculoskeletal Antagonistic Joints

Amirhossein Kazemipour [1], Ronan Hinchet [1], Robert K. Katzschmann [1]

[1] Soft Robotics, D-MAVT, ETH Zurich

22 **Enrriquez Casimiro Nadia** **CONFIDENTIAL**

Bacteria-driven Precipitation of Calcium Carbonate in Droplets

Nadia Enrriquez Casimiro [1], Carla Fernández-Rico [1], Elena Tervoort [1], Julie M. Laurent [1], André R. Studart [1]

[1] Complex Materials, D-MATL, ETH Zurich

23 **Kindler Robert Oswin** **CONFIDENTIAL**

Exploring Living Organisms for Wood-Based Materials

Robert O. Kindler [1], Elena Passaretti [1], Laura Stricker [1], Guido Panzarasa, and Ingo Burgert

[1] Wood Materials, D-BAUG, ETH Zurich

24 **Kiwic David** (non-confidential)

Nanoparticle Gelation at Tailored pH For Advanced Photocatalysts

David Kiwic [1], Markus Niederberger [1]

[1] Multifunctional Materials, D-MATL, ETH Zurich

Nanoparticle gelation offers a pathway to create highly crystalline, translucent aerogels with extensive surface areas. A key prerequisite for successful nanoparticle gelation is achieving colloidal dispersion at relatively high particle concentrations. Current methodologies for TiO_2 nanoparticle gelation necessitate harsh acidic conditions, constraining the range of compatible materials. In contrast, our novel approach utilizes organic ligands to facilitate nanoparticle dispersion under mild conditions in water. Trisodium citrate serves as an effective ligand to functionalize TiO_2 nanoparticles, yielding stable colloidal dispersions across a broad pH spectrum (pH 3-12). These dispersions can be gelled and extruded to form solvo-gel granules, subsequently super-critically dried to yield translucent aerogel granules. This innovation enables the co-gelation of a wider range of materials, allowing their incorporation into the aerogel under pH conditions tailored to their requirements.

Moreover, we employed titanium-isopropoxide as a precursor for TiO_2 synthesis, departing from the conventional chloride precursor (titanium tetrachloride), thus eliminating chlorides from the process. To illustrate the versatility of these nanoparticle building blocks, we successfully produce highly translucent silver (Ag) on TiO_2 aerogels, showcasing exceptional dispersion of co-gelled nanoparticles throughout the aerogel matrix. The choice of Ag showcases the utility of our chloride-free, mild pH approach, as conventional chloride-derived TiO_2 particles may lead to corrosion and precipitation of the Ag nanoparticles.

Furthermore, the Ag/TiO_2 composite aerogel exhibits photocatalytic activity for the reduction of CO_2 to CO by H_2, a pivotal reaction for producing renewable feedstocks in the chemical industry. Our chloride-free methodology holds significant promise for tailoring materials for diverse applications, particularly in (photo-)catalysis and optical materials.

25 **Lohmann Victoria** **CONFIDENTIAL**

Chemical recycling of poly(methacrylamides): low temperature depolymerization of biorelevant polymers

Victoria Lohmann [1], Glen R. Jones [1], Asja Kroeger [2], Nghia P. Truong [1], Michelle Coote [2], and Athina Anastasaki [1]

[1] Polymeric Materials, D-MATL, ETH Zurich
[2] Institute for Nanoscale Science and Technology, College of Science and Engineering, Flinders University

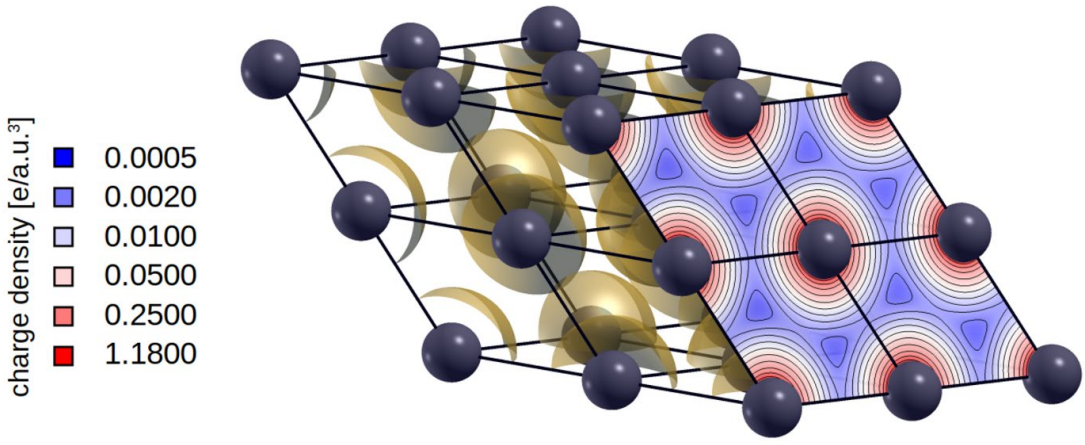
26 **Marin Luca** (non-confidential)

Description of Dark Matter-Electron Scattering in Liquid Xenon Targets via Density Functional Theory

Luca Marin [1], Marek Matas [1], Einar Urdshals [2], Riccardo Catena [2], and Nicola A. Spaldin [1]

[1] Materials Theory, D-MATL, ETH Zurich
[2] Department of Physics, Chalmers University of Technology, Sweden

We explore the effect of the interatomic interactions in the condensed phases of xenon on the dark matter-electron scattering process, with a focus on applications in liquid xenon detectors. We calculate the electronic structure of atomic, liquid and solid xenon using first-principles density functional theory (DFT) and then compute material response functions for the dark matter-electron scattering process within an effective field theory framework. Finally, we use experimental data from XENON10 and XENON1T experiments to compare exclusion limits obtained for isolated atoms and for the condensed phase. Our results allow us to assess the impact of the interatomic interactions on dark matter-electron scattering in liquid xenon.



Charge density isosurfaces (yellow blobs, isovalue of 0.015 e/a.u.^{3}) and contour plot of solid crystalline xenon within the (111) plane.

27 **Medany Mahmoud** **CONFIDENTIAL**

Ultrasound Microrobots Navigate Against the Flow Using Model-Based Reinforcement Learning

Mahmoud Medany [1], Lorenzo Piglia [1], Liam Achenbach [1], S. Karthik Mukkavilli [2], Daniel Ahmed [1]

[1] Acoustic Robotics System, D-MAVT, ETH Zurich
[2] IBM Research, AI and Accelerated Discovery

28 **Mlkvik Peter** (non-confidential)

Metal-insulator Transition in VO2 within a Bond-centered Approach

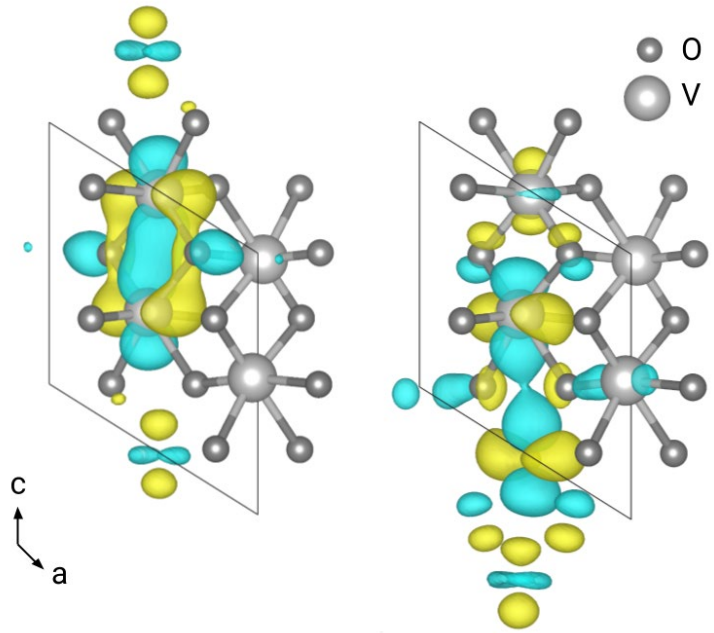
Peter Mlkvik [1], Maximilian E. Merkel [1], Nicola A. Spaldin [1], and Claude Ederer [1]

[1] Materials Theory, D-MATL, ETH Zurich

Vanadium dioxide (VO_2) is a prototypical material undergoing a metal-insulator transition (MIT), hosting both intriguing physical phenomena and the potential for industrial applications. The coupled structural and electronic transition in VO_2 has been a topic of a long-standing discussion, with much of the work focused on methods for correctly simulating the physics of the material. In our work [1], we present an unconventional set of bond-centered orbitals studied within *ab initio* density-functional theory and dynamical mean-field theory calculations. With our choice of basis, we investigate the interplay of structural dimerization and electronic correlations in VO_2 in a computationally cheaper way than the other state-of-the-art methods. Our approach also allows us to, for the first time, vary the distortion across the MIT and observe the transition in detail. The choice of basis hence offers a complementary view on the long-standing discussion of the MIT in VO_2 and suggests possible future extensions to other similar materials hosting molecular-orbital-like states.

[1] P. Mlkvik, M. E. Merkel, N. A. Spaldin, and C. Ederer, arXiv:2402:12798 (2024).

Bond-centered orbitals of VO_2 used in this work



29 **Pereira Martins Michael** **CONFIDENTIAL**

Template-free and dry synthesis of highly porous metal nitride architectures for electronics and molecular sensing

Michael Pereira Martins [1], Adrien Baut [1], Andreas T. Güntner [1]

[1] Human-centered Sensing, D-MAVT, ETH Zurich

30 **Porenta Nikolaus** (non-confidential)

Composition Control of Alloy Fabrication Using Localized Electrochemical Deposition for Small-Scale Additive Manufacturing

Nikolaus Porenta [1], Mirco Nydegger [1], Souzan Hammadi [1,2], Alain Reiser [1,3], and Ralph Spolenak [1]

[1] Nanometallurgy, D-MATL, ETH Zurich
[2] Currently at: Uppsala University, Structural Chemistry Division, Department of Chemistry, Ångström Laboratory
[3] Currently at: KTH, Department of Material Science and Engineering

Alloying different metals has proven effective in optimizing material properties, including mechanical strength, plasmonic resonances, and corrosion resistance. Achieving precise control over the chemical composition of alloys is of paramount importance for many applications. However, several sub-micron resolution additive manufacturing techniques face challenges in fabricating a wide range of compositions. In this study, we leverage droplet-confined electroplating through electrohydrodynamic printing (EHD-RP) to develop a range of alloys that can be deposited into 3D geometries. Using aqueous mixed metal salt solutions, we demonstrate the ability to precisely control the composition of fabricated alloys. Microstructural investigation reveals a kinematically controlled deposition process. Nanoporous Ag with ligaments <100nm can be produced from our fabricated CuAg alloys, showing promising potential for surface-enhanced Raman spectroscopy applications. This innovative approach offers a pathway towards the development of tailored alloys with controlled compositions using small-scale additive manufacturing methods.

31 **Pozzi Marcello** **CONFIDENTIAL**

Symmetry breaking in plasmonic meta-atoms based on quantum graphs

Jelena Wohlwend [1], Marcello Pozzi [1], Philipp del Hougne [2], Georg Haberfehlner [3], Ralph Spolenak [1], Henning Galinski [1]

[1] Nanometallurgy, D-MATL, ETH Zurich
[2] CNRS, University Rennes
[3] Institut für Electronenmikroskopie und Nanoanalytik, TU Graz

32 **Prountzou Eleni** (non-confidential)

Fabrication and Characterization of Polycrystalline Barium Titanate Films for Integrated Quantum Devices

Eleni Prountzou[1], Ülle-Linda Talts[1], Helena C. Weigand[1], Irene Occhiodori[1], Virginia Falcone[1], Elise Bailly[1], and Rachel Grange[1]

[1] Optical Nanomaterials, D-PHYS, ETH Zurich

Barium titanate ($BaTiO_3$, or BTO) is known for its versatile nonlinear optical properties, second-harmonic generation (SHG) [1], electro-optic effect, and ferroelectric characteristics. While various techniques such as MBE, MO-CVD, and PLD have been explored for BTO film fabrication, challenges like the need for specialized equipment, the formation of orthogonal crystalline domains, and limitations in substrate materials have obstructed the commercialization of BTO thin films. The sol-gel process emerges as a cost-effective and scalable approach for producing polycrystalline BTO films, offering significant potential for tailoring material properties to meet specific demands.

Our research focuses on optimizing the sol-gel fabrication process to enhance film quality and properties. Notably, we have made significant progress in determining optimal conditions for inter-layer calcination (i.e., the annealing process occurring between successive layers of the spin-coated material), precursor concentration, and final annealing temperature control, which are crucial factors in the production of high-quality BTO films. We determine that a pyrolysis at 450°C between every single-layer (~ 30 nm thick) spin-coated yields highest crystallinity and lower surface roughness. Additionally, optimization studies unveiled the significant impact of solution concentration on film characteristics and stability. Specifically, we tested four different concentrations, and we observed that higher concentrations led to thicker films with larger grains but also introduced challenges such as solution instability and impurity formation. Furthermore, systematic investigation of the final annealing temperature (600 – 1000ºC) demonstrated temperature-dependent grain growth and crystallinity, alongside tendencies for impurity formation. While higher temperatures (> 800ºC) enhanced crystallinity and reduced porosity, they also correlated with the appearance of impurity peaks, highlighting the importance of precise temperature control in the fabrication process.

[1] Ü. Talts, H. C. Weigand, G. Saerens, P. Benedek, J. Winiger, V. Wood, J. Leuthold, V. Vogler-Neuling, R. Grange, Sol–Gel Barium Titanate Nanohole Array as a Nonlinear Metasurface and a Photonic Crystal. Small 2023, 19, 2304355. https://doi.org/10.1002/smll.202304355

33 **Reiter Manuel** **CONFIDENTIAL**

Controlled Halogenation of the Solid Electrolyte Interphase in Li Metal Batteries

Manuel Reiter [1], Maria R. Lukatskaya [1]

[1] Electrochemical Energy Systems, D-MAVT, ETH Zurich

34 **Rich Andrea** (non-confidential)

In vivo sensors to characterize Mg and Ti implants

Andrea M Rich [1], Wolfgang Rubin [1], Stefan Rickli [2], Tatiana Akhmetshina [1], Leopold Berger [1], Katja Nuss [3], Benoit Schaller [4], Jörg F. Löffler [1]

[1] Metal Physics and Technology, D-MATL, ETH Zurich
[2] Center for Project Based Learning, D-ITET, ETH Zurich
[3] Musculoskeletal Research Unit, University of Zurich
[4] Inselspital, Bern University Hospital

Mechanical and environmental parameters (temperature, pH) affect magnesium degradation [1,2], but little is currently known about the exact *in vivo* conditions [3]. Limited mechanical loading data exists, though this has strong implications for implant design and fracture healing [4]. To address these shortcomings, we developed a fully-implantable measurement system to record temperature, pH, 3D movement, and strain *in vivo*. The measurements were performed on magnesium and titanium plates, fixating bilateral zygomatic arch fractures in three female alpine sheep for 8 weeks. No strong trend can be seen regarding temperature, indicating no localized temperature increase during fracture healing. The pH above the Mg plates shows a trend towards higher pH compared to Ti, though not higher than expected for normal blood pH. Strain readings allow determination of dynamic loading that the plates experience during chewing. These results show that it is possible to record environmental and mechanical factors that may affect biodegradable implants *in vivo* continuously, enhancing the understanding of these alloys and allowing for improvements in clinical applications.

[1] J. Gonzalez et al., Adv. Healthcare Mater. 10, 2100053 (2021)
[2] C. Wang et al., Corr. Sci. 197, 110059 (2022)
[3] A.H.M Sanchez, et al., Acta Biomater. 13, (2015)
[4] L. Claes, J. Biomech. 115, 110148 (2021)

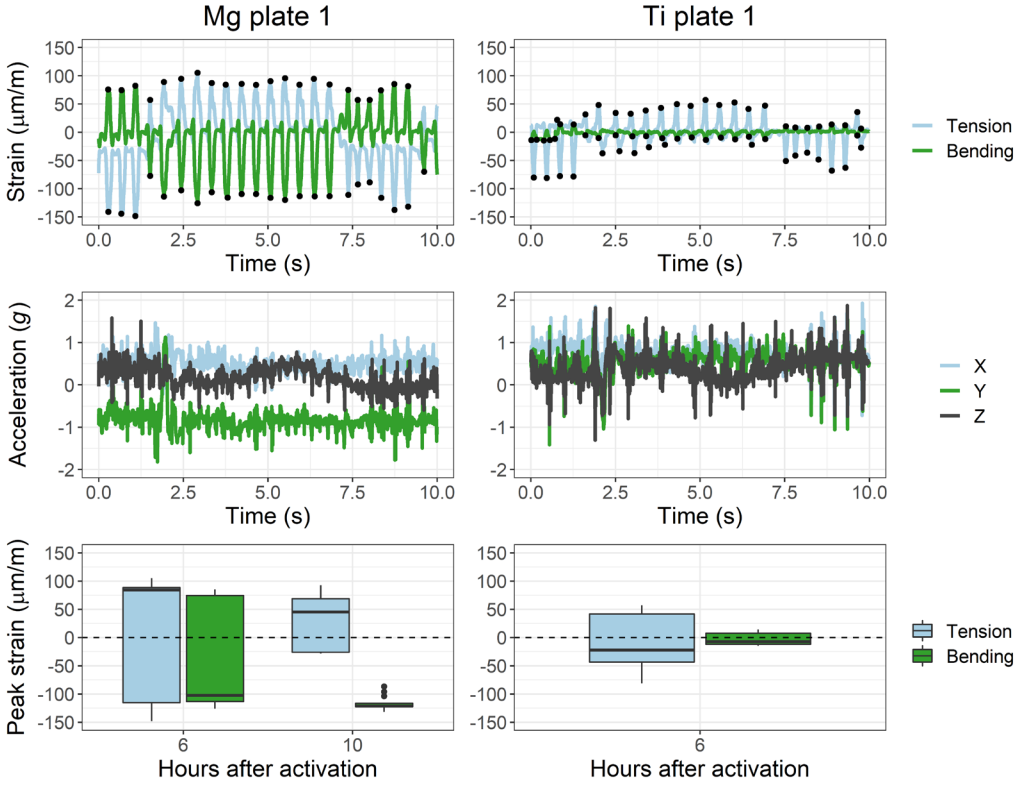


Fig. 1: Data recorded six hours after implantation during dynamic loading (chewing). Peak strains were calculated (black points) for each loading direction

35 **Schenk Florian** (non-confidential)

Phase-change memory from molecular tellurides

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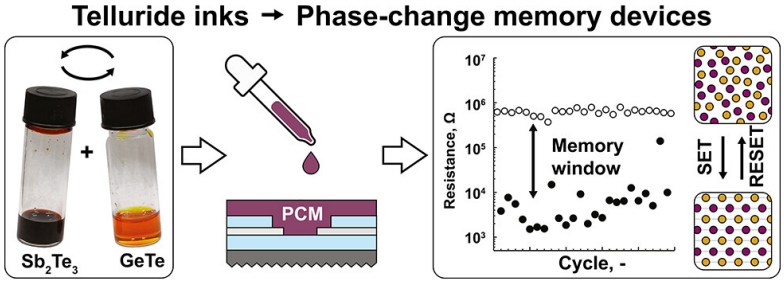
Phase-change memory (PCM) is an emerging memory technology based on the resistance contrast between the crystalline and amorphous states of a material. It possessed great potential for faster RAM or brain-like neuromorphic for enhanced artificial intelligence applications. Further development of PCM as a mainstream memory technology relies on innovative materials and inexpensive fabrication methods. Here, we propose a generalizable and scalable solution-processing approach to synthesize phase-change telluride inks in order to meet demands for high-throughput material screening, increased energy efficiency, and advanced device architectures. Bulk tellurides, such as Sb2Te3, GeTe, Sc2Te3, and TiTe2, are dissolved and purified to obtain inks of molecular metal telluride complexes. This allowes us to unlock a wide range of solution-processed ternary tellurides by the simple mixing of binary inks. We demonstrate accurate and quantitative composition control, including prototype materials (Ge−Sb−Te) and emerging rare-earth-metal telluride-doped materials (Sc−Sb−Te). Spin-coating and annealing convert ink formulations into high-quality, phase-pure telluride films with preferred orientation along the (00l) direction. Deposition engineering of liquid tellurides enables thickness-tunable films, infilling of nanoscale vias, and film preparation onflexible substrates. Finally, we demonstrate cyclable and non-volatile prototype memory devices, achieving a resistance contrast and low reset energy on par with state-of-the-art sputtered PCM layers.



37 **Scherrer Simon** (non-confidential)

Characterising Rough and Adhesive Single-Particle Contacts

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The rheological response of particulate suspensions plays a crucial role in both natural and industrial settings. In particular, suspensions in which the viscosity increases non-linearly above a critical shear stress (shear thickening suspensions) have been studied extensively. The origin of this phenomenon can be traced back to the emergence of constraints in the relative motion between the particles, which can be induced by turning on frictional and adhesive interactions. Characterizing contacts during rolling motion remains extremely challenging, since it is not possible with commonly employed colloidal-probe atomic force microscopy. To address this issue, we present a new approach: a particle in a liquid is captured by a custom nano-fabricated holder attached to a conventional AFM cantilever and translated horizontally. The studied particles are optically anisotropic to quantitatively track particle rotation, while simultaneously measuring the normal and lateral forces. Using surface-modified silica particles, we demonstrate that an increase in adhesion or roughness at the contact induces the particles to transition from sliding to rolling motion. Notably, the rolling mechanisms qualitatively differ between rough and adhesive substrates, due to the different origin of traction at the contact. In general, the friction experienced by a rolling particle is significantly lower than a sliding particle, while the average contact duration increases. With this technique, we can study contacts akin to those formed in dense particulate suspensions under shear, paving the way for the design of custom surfaces to control the rheology in shear-thickening materials and beyond.

38 **Seda David** (non-confidential)

Nanoimprint Lithography of Optical Fourier Surfaces

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Grayscale patterning of optical Fourier surfaces [1] using thermal scanning-probe lithography (t-SPL) allows for continuous, nanometer depth control and high spatial resolution at the required precision. Nevertheless, this technique exhibits some limitations for advancing the fabrication process of Fourier surfaces (FS). Current tools need considerable time to write multiple patterns. Nanoimprint lithography [2] (NIL) provides a suitable technique for overcoming these limited writing speeds by mass reproducing such grayscale patterns. Thermal nanoimprint lithography was shown to be a suitable process for the large-scale fabrication of Fourier surfaces. Once the patterns have been imprinted into PMMA, they can be either etched into materials such as Si or transferred to other materials such as Ag using template stripping [3]. Although preliminary experiments using OrmoStamp® for UV NIL [4] have shown some slight loss in pattern amplitude, it seems to be a simple and promising method to produce molds for nanoimprinting. Fully covering a larger surface with Fourier surfaces using NIL is currently still being investigated. Large-scale fabrication of Fourier surfaces is essential in many applications, such as holography.

[1] Lassaline et al., Nature 582, 506 (2020)
[2] Chou et al., Appl. Phys. Lett. 67, 3114 (1995)
[3] Nagpal et al., Science 325, 594 (2009)
[4] Kulmala et al., Novel Patterning Technol. 10584, 1058412 (2018)

39 **Sifringer, Léo** (non-confidential)

Interfacing Soft Electronics and Engineered Neuronal Networks: a Nerve-on-a-Chip Model Towards Biohybrid Electronics

Léo Sifringer [1], Alex Fratzl [2], Blandine Clément [1], Parth Chansoria [4], Leah Mönkemöller [1], Jens Duru [1], Stephan J. Ihle [1], Simon Steffens [1], Anna Beltraminelli [1], Eylul Ceylan [1], Benedikt Maurer [1], Sean Weaver [1], Christina M. Tringides [1], Katarina Vulić [1], Srinivas Madduri [3], Marcy Zenobi-Wong [4], Botond Roska [2], János Vörös [1] and Tobias Ruff *[1]

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In this work, we introduce a novel nerve-on-a-chip model designed as a neural interface for deep brain stimulation. Termed as a "biohybrid" approach, it aims to overcome the limitations of standard deep brain implants such as low stimulation resolution. The biohybrid concept leverages on-chip grown neurons to convert electrical signals from a stretchable 2D multielectrode array (MEA) into synaptic stimulation of a neural target tissue (Figure 1C).

The device (Figure 1A) consists of two primary components: a soft, stretchable MEA and an axon-guiding microstructure [1]. Spheroids of retinal neurons are then seeded into the device for culturing and subsequent device implantation.

We describe the fabrication of the biohybrid neural interface and demonstrate how the neurons seeded into the implant form an artificial nerve *in vitro* (Figure 1B) and *in vivo*. We show that spheroids can be stimulated using the stretchable MEA, and exhibit spontaneous activity for over 3 weeks when implanted in mice.

Further experiments are necessary for in vivo synapse formation and deep-brain stimulation, but previous work has shown feasibility of this approach in vitro [2].

[1] C. Forró et al., Biosens. Bioelectron. 122:7587 (2018)
[2] G. Amos et al., Front. Neurosc. 14 (2024)

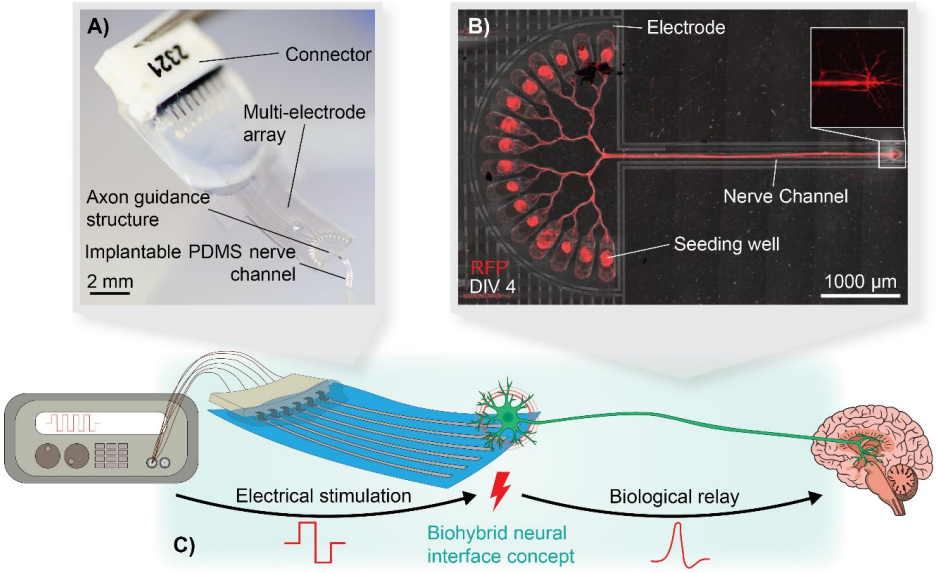

Figure 2: Overview of the biohybrid neural interface. A) Photograph of the device. The device consists of a stretchable multi-electrode array and a PDMS microstructure in which neurons can be seeded. B) Fluorescent imaging of neurons growing in the device, forming an artificial nerve-like structure. C) Conceptual schematic of the biohybrid interface: neurons grown on the devices are electrically stimulated and are aimed to be used as biological relays to stimulate a target structure (e.g. deep brain stimulation)

40 **Simmen Edith** (non-confidential)

Interplay of metallicity, ferroelectricity and layer charges: A DFT study of SmNiO3 and BaTiO3 superlattices

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We present a density functional theory (DFT) study of superlattices containing metallic $SmNiO_3$ (SNO) and ferroelectric $BaTiO_3$ (BTO). The interface of SNO with BTO hosts numerous interesting functionalities which can compete or cooperate: Since BTO and SNO are II-IV and III-III perovskites, respectively, the different layer charges lead to a built-in polar discontinuity in addition to the spontaneous polarization of BTO. These two sources of polarization can both interact with each other and with the SNO via its metallic screening. We find that despite the metallicity of SNO, the polar electrostatics strongly affect the ground state. The system avoids a polar discontinuity by aligning the spontaneous polarization of the BTO parallel to the layer polarization of the SNO in the so-called 'happy' orientation. We find that this happy polarization is stable down to a single unit cell of BTO, in contrast to the 6-unit-cell critical thickness previously found for BTO with II-IV metallic electrodes [1]. The opposite 'unhappy' polarization orientation is however highly unfavoured, with the stability depending strongly on the thickness of the BTO layer and the tilts within the SNO layer.

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41 **Smid Caroline** (non-confidential)

Buckling-Inspired Heart Valve Leaflet Designs for Stiff Polymeric Materials

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Despite continuous efforts to improve robustness of cardiac valve implants, neither bioprosthetic, nor mechanical valves fulfill both hemodynamic and durability requirements. This study presents novel flexible leaflet designs, focusing on polymeric materials with proven hemocompatibility, such as PEEK, of much higher stiffness than native tissue, aiming on optimal valve implants. A biomimetic valve with a single-curvature belly-curve serves as reference for the new design variants with a double-curvature belly-curve with varying radii. Soft (13.2 MPa), as well as stiff (2.4 GPa) leaflet materials, and different thicknesses are studied by means of lean simulations, and in-vitro experiments under physiologic hemodynamic conditions. The performance is assessed by opening pressure and orifice area. The latter is determined by a newly developed automatized image processing tool. Experimental trends are in agreement with simulations and demonstrate that a buckling inspired, double-curvature leaflet design, significantly enhances tri-leaflet valves' opening behavior, particularly advantageous for stiffer leaflet materials. Best performing variant shows an opening pressure improvement in the range of 47% and 44% based on simulations and experiments, respectively, compared to reference, while achieved mean pressure differential is directly comparable to state-of-art bioprosthetic valves. The orifice area is slightly reduced for new variants, yet still in satisfying range.

42 **Song Chao** (non-confidential)

Droplet-based Fabrication of Soft Microrobots with Tailored Magnetic Anisotropy

Chao Song [1], Yimo Yan [2], Michael G. Christiansen [2], Stavros Stavrakis [1], Simone Schürle [2] and Andrew deMello [1]

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We present a method for the high-throughput fabrication of magnetically anisotropic soft microrobots by integrating droplet-based microfluidics and magnetron control. Soft microrobots are finding widespread applications in targeted drug delivery, biosensing, and diagnostics. Unfortunately, traditional methods like micromachining and additive manufacturing are unsuitable for mass production. [1]. Conversely, droplet-based microfluidic systems are able to generate user-defined micron-sized objects at high-throughput [2]. Based on these advantages, we combine microfluidics with precise magnetic manipulation, to enable the efficient and large-scale fabrication of soft robots with bespoke magnetic properties. As shown in Figure 1, we are able to generate diverse magnetic anisotropy configurations by the controlled distribution of magnetic beads within droplets. Solidifying droplets without a magnetic field creates microrobots with uniform bead distribution. Solidifying in a uniform magnetic field forms chain-like or bundle-shaped distributions, while crosslinking under a rotating magnetic field results in disk-like distributions. Such distinct and controllable distributions of magnetic beads significantly impact the behavior of soft microrobots in various scenarios.

[1] Sungwoong Jeon, et. al., Sci. Robot. 4, eaav4317 (2019).
[2] Xie M, et. al., Adv. Mater. 32, 2000366 (2020).

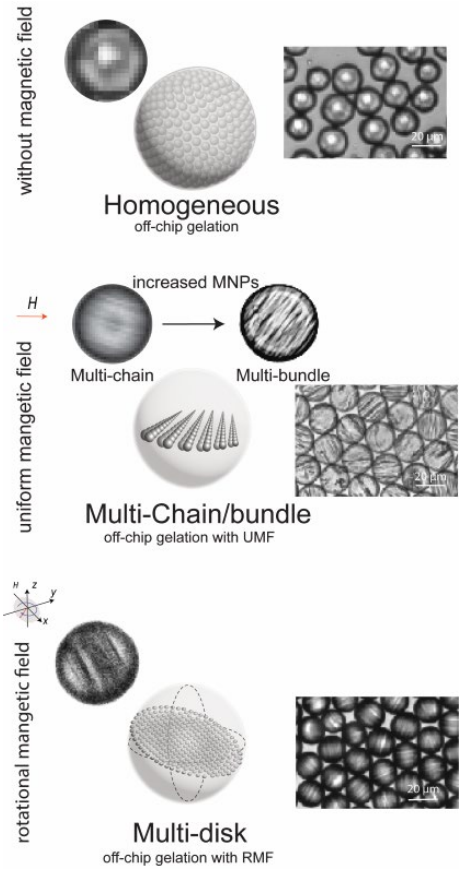

Figure 1: Distinct magnetic supradomain are generated under the application of different magnetic fields.

43 **Stanko Štefan T.** (non-confidential)

Structural and Thermal Characterization of Zr-Based Bulk Metallic Glasses via Fast Differential Scanning Calorimetry and Synchrotron X-Ray Diffraction

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Bulk metallic glasses (BMGs) are metallic alloys with a disordered atomic arrangement, obtained via rapid cooling from the melt. They often exhibit unique engineering properties and form multiple complex phases. MEMS chip-based fast differential scanning calorimetry (FDSC) can be used to study the formation of metallic glasses, their stability and the kinetics of phase transformations due to the high heating and cooling rates achievable with FDSC. In this context, a simultaneous combination of calorimetric and structural characterization techniques is of great advantage. We thus modified a fast differential scanning calorimeter to enable its integration into a synchrotron X-ray beamline and characterize *in situ* metastable phase transformations. For this purpose, the FDSC external sensor support was placed vertically in the beam path. An opening was drilled at the bottom side of the sensor to allow the X-ray beam to reach the sample. Both sides were closed by a polyimide window and the furnace was purged with argon to prevent sample oxidation. This setup enables the simultaneous study of the structure and thermophysical properties of materials, which was demonstrated on Zr-based BMGs used for additive manufacturing.

The alloys were also characterized *ex situ* in powder and bulk form. Critical cooling and heating rates and time-temperature-transformation (TTT) diagrams were measured and multiple crystallization events upon cooling were observed in both cases. The results are discussed with respect to the oxygen content of the samples with the aim of optimizing the additive manufacturing process of metallic parts.

44 **Veciana Andrea** **CONFIDENTIAL**

Breaking the PFAS Chain: Piezocatalytic Decomposition of Forever Chemicals Using $BaTiO_3$ Nanoparticles

Andrea Veciana [1], Sarah Steiner [1], Qiao Tang [1], Vitaly Pustovalov [1], Joaquim Llacer [1], Jiang Wu [1], Xiang-Zhong Chen [2], Trust Manyiwa [3], Venecio U. Ultra Jr. [3], Beltzane Garcia-Cirera [4], Josep Puigmartí-Luis [4], Carlos Franco [1], David J. Janssen [5], Laura Nyström [6], Samy Boulos [6], Salvador Pané [1]

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[4] Departament de Ciència de Materials i Química Física, Universitat de Barcelona
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[6] Food Biochemistry, D-HEST, ETH Zurich

45 **Wang Hanchen** (non-confidential)

Understanding the Magnetic Properties of Ultrathin BiYIG Grown by Sputtering

Hanchen Wang [1], W. Legrand [1], R. Schlitz [1], M. Lammel [2], M. H. Aguirre [3], P. Gambardella [1]

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Ferrimagnetic insulator thin film garnets with perpendicular magnetic anisotropy have recently expanded the realm of experimental possibilities in magnonics (e.g., [1]). Even though several rare-earth doped and substituted garnet compositions (from Ce to Tm) have been investigated for their perpendicular magnetization, thin films of LuIG [2], YIG [3] and Bi-doped YIG (BiYIG) [4] remain the only compositions enabling a damping in the 10-4 range, required for many types of experiments. Among these low-damping garnets, perpendicular magnetic anisotropy has been more practically achieved with BiYIG.
We cover in this contribution our recent progress in the growth by magnetron sputtering of ultrathin BiYIG films with tunable magnetic anisotropy and low damping. The thickness of BiYIG investigated in this work ranges within 3-30 nm. We study the degree of crystalline perfection, the strain, the elemental composition and its thickness dependence, as well as the dynamical magnetic properties of BiYIG, by X-ray characterization, TEM imaging, analytical techniques in SEM and TEM, ferromagnetic resonance measurements and non-local magnon transport experiments. We relate the evolution of these properties to some of the deposition parameters, essentially sputtering gas mixture and deposition power, in the aim of providing useful guidelines for future works with this system.
As expected from strain-related magnetocrystalline anisotropy and growth-induced anisotropy in epitaxial conditions, the choice of the substrate [4] and deposition conditions [5] allows to tune the magnetic anisotropy with precision across the magnetic reorientation. We find that the sputter-grown films differ from films grown by pulsed laser deposition in several aspects. This establishes further BiYIG as an ideal platform to combine studies relating to spin-pumping, incoherent spin-waves diffusion and coherent spin-waves propagation.

[1]Y. Fan et al., arXiv: 2212.01408
[2]C. L. Jermain et al., Appl. Phys. Lett. 109, 192408 (2016)
[3]J. Ding et al., Phys. Rev. Appl. 14, 014017 (2020)
[4]L. Soumah et al., Nat Commun. 9, 3355 (2018)
[5]D. Gouéré et al., Phys. Rev. Materials 6, 114402 (2022)

46 **Winters Arturo** (non-confidential)

Pioneering Fluctuations in Viscoelastic Stress: A Comparison of the Temporary Network and Dumbbell models

Arturo Winters [1], Jan Vermant [1]

[1] Soft Materials, D-MATL, ETH Zurich

Traditionally, stress fluctuations in flowing and deformed materials are overlooked, with an obvious focus on average stresses in a continuum mechanical approximation. However, these fluctuations, often dismissed as “noise”, hold the potential to provide direct insights into the material structure and its structure-stress coupling, uncovering detailed aspects of fluid transport and relaxation behaviors. Despite advancements in experimental techniques allowing for the visualization of these fluctuations, their significance remains largely untapped, as modeling efforts continue to target Newtonian fluids within the confines of Gaussian noise assumptions. This talk presents the work [1], which entails a comparative analysis of stress fluctuations in two distinct microstructural models: the temporary network model and the dumbbell model. Despite both models conforming to the Upper Convected Maxwell Model at a macroscopic level, the temporary network model predicts non-Gaussian fluctuations. We find that stress fluctuations within the temporary network model exhibit more pronounced abruptness at local scale, with only an enlargement of the control volume leading to a gradual Gaussian-like noise, diminishing the differences between the two models. These findings underscore the heightened sensitivity of fluctuating rheology to microstructural details and the microstructure-flow coupling, beyond what is captured by macroscopically averaged stresses.

[1] A. Winters, H. C. Öttinger, J. Vermant, arXiv:2404.19743, (2024)

47 **Wintersteller Simon** (non-confidential)

Unravelling the Amorphous Structure and Crystallization Mechanism of GeTe Phase Change Memory Materials

Simon Wintersteller [1], Olesya Yarema [1], Dhananjeya Kumaar [1], Florian M. Schenk [1], Olga Safonova [2], Paula M. Abdala [3], Vanessa Wood [1], Maksym Yarema [1]

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The reversible phase transitions in phase-change memory devices can switch on the order of nanoseconds, suggesting a close structural resemblance between the amorphous and crystalline phases. Despite this, the link between crystalline and amorphous tellurides is not fully understood nor quantified. Here we use in-situ high-temperature x-ray absorption spectroscopy (XAS) and theoretical calculations to quantify the amorphous structure of bulk and nanoscale GeTe. Based on XAS experiments, we develop a theoretical model of the amorphous GeTe structure, consisting of a disordered fcc-type Te sublattice and randomly arranged chains of Ge atoms in a tetrahedral coordination. Strikingly, our intuitive and scalable model provides an accurate description of the structural dynamics in phase-change memory materials, observed experimentally. Specifically, we present a detailed crystallization mechanism through the formation of an intermediate, partially stable 'ideal glass' state and demonstrate differences between bulk and nanoscale GeTe leading to size-dependent crystallization temperature. Finally, we study the influence of nanoparticle surfaces and the effects of spatial confinement, on the lattice stress and atomic mobility of the structure. We investigate how this influences the crystallization dynamics, specifically the speed of Te preordering and the stability of the 'ideal glass' state prior to complete crystallization.

[1] S. Wintersteller, et. al., Nat Commun 15, 1011 (2024)

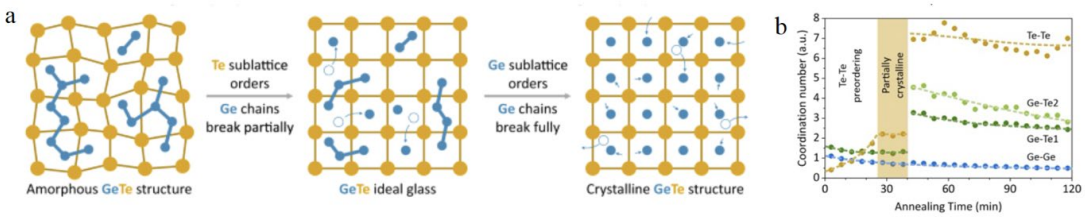

Figure 1. Crystallization mechanism of bulk GeTe: (a) graphical depiction and (b) bond coordination.

48 **Wolfisberg Gianna (& Bittmann Pablo Camilo)** (non-confidential)

Impact of Induced Spontaneous Curvature on the Shape of Adhered, Phase Separated Pancake-like GUV's and Their Digital Reconstruction as a Mesh

Pablo C. Bittmann [1], Gianna C. Wolfisberg [1], Jaime Agudo-Canalejo [2], Robert W. Style [1], Jan C. Vermant [1], and Aleksander A. Rebane [1,3]

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Giant unilamellar vesicles (GUVs) are artificial bilayer compartments that are suitable to model biological organelles with large surface to volume ratios, what we achieve through the adhesion and deflation of GUVs on a supported lipid bilayer. Biological membranes have a complex bilayer composition that may differ across the surface and likely has an influence on the shape of the membrane. Here, we study phase separating GUVs consisting of DOPC, DPPC and cholesterol at different ratios made by electroformation to see whether the shape of the vesicle depends on the phase distribution. We find that in all our samples, the driving force of curvature optimization is too low to induce a phase separation. If a temperature induced phase separation takes place, a phase ordering - presumably based on curvature - can be observed. The DPPC rich phase stays in the low curvature region of the adhesion zone, whereas the DOPC rich phase is found at the adhesion rim and cupola of the vesicle. Furthermore, we observe bending and budding of phases due to line tension as well as jamming of phases.

Complementary, we develop a program to digitally reconstruct phase separated, deflated GUVs from confocal microscopy z-stacks in the form of a mesh. It includes analysis on the shape of the mesh regarding geometrical measures and is capable of mapping curvature as well as colors from confocal microscopy stack on the mesh.

49 **Xie Chang** (non-confidential)

High-efficient Engineering of Osteo-callus Organoids for Rapid Bone Regeneration Within One Month

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Large bone defects that cannot form a callus tissue are often faced with long-time recovery[1]. Developmental engineering-based strategies with mesenchymal stem cell (MSC) aggregates have shown enhanced potential for bone regeneration[2]. However, MSC aggregates are different from the physiological callus tissues, which limited the further endogenous osteogenesis. This study aims to achieve engineering of osteo-callus organoids for rapid bone regeneration in cooperation with bone marrow-derived stem cell (BMSC)-loaded hydrogel microspheres (MSs) by digital light-processing (DLP) printing technology and stepwise-induction. The printed MSC-loaded MSs aggregated into osteo-callus organoids after chondrogenic induction and showed much higher chondrogenic efficiency than that of traditional MSC pellets. Moreover, the osteo-callus organoids exhibited stage-specific gene expression pattern that recapitulated endochondral ossification process, as well as a synchronized state of cell proliferation and differentiation, which highly resembled the diverse cell compositions and behaviors of developmentally endochondral ossification. Lastly, the osteo-callus organoids efficiently led to rapid bone regeneration within only 4 weeks in a large bone defect in rabbits which need 2–3 months in previous tissue engineering studies. The findings suggested that in vitro engineering of osteo-callus organoids with developmentally osteogenic properties is a promising strategy for rapid bone defect regeneration and recovery.

[2] Liu, Yuwei et al., Biomaterials vol. 218 (2019): 119336.
[2] Nilsson Hall, Gabriella et al.,Adv Sci (Weinh). 2019 Dec 10;7(2):1902295.

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