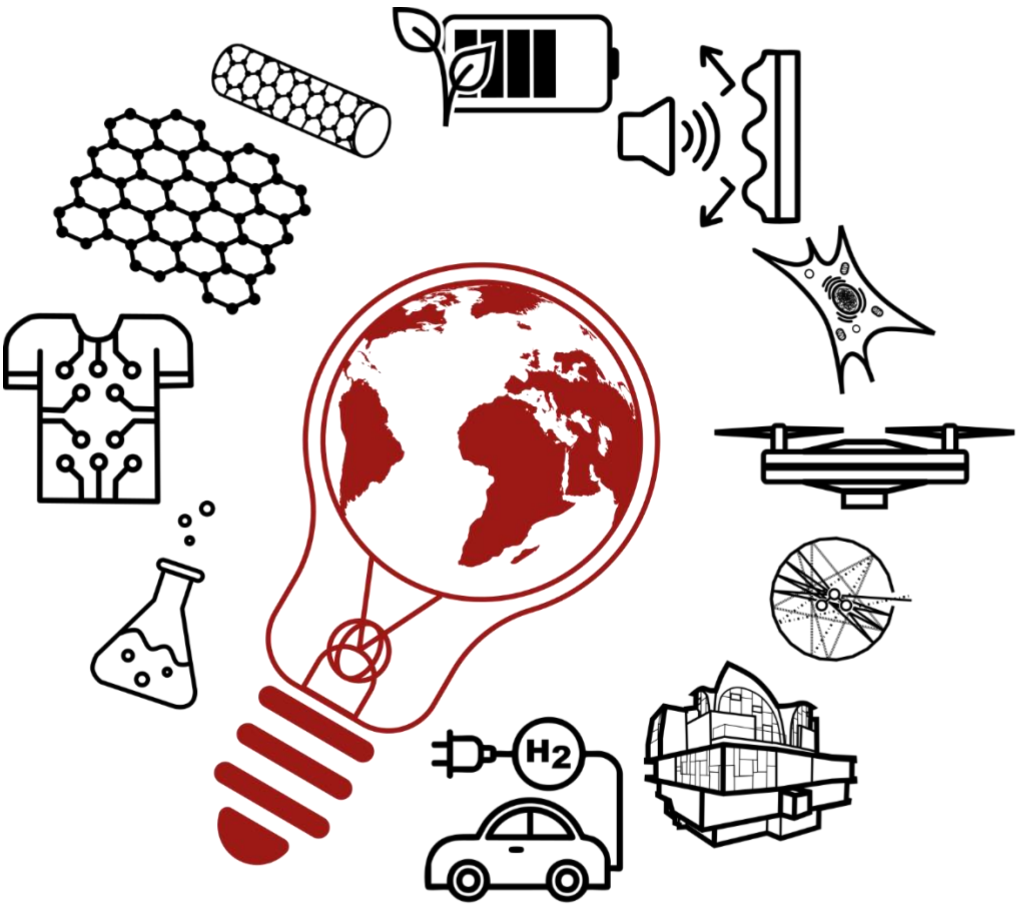


Empa PhD Symposium 2025

"Illuminating the world"

Driving industry innovation through impactful research

27.02.2025, Empa Akademie, Überlandstrasse 129, 8600 Dübendorf

The Organizing Committee

Anna-Lena Bauknecht - *Biointerfaces*

Christopher Bascucci - *High Performance Ceramics*

Dominique Grimm - *Biomimetic Membranes and Textiles*

Hyunjoo Hong - *Technology and Society*

Mariia Svyrydenko - *Thin Films and Photovoltaics*

Michelle Jessy Müller - *Air Pollution / Environmental Technology*

Reshma Peremadathil Pradeep - *Magnetic and Functional Thin Films*

Program Overview

08:00 – 08:30	**Registration and coffee**	
08:30 – 08:45	Tanja Zimmermann	*Opening*
08:45 – 09:00	Melina Spycher	*Diversity and Inclusion*
09:00 – 09:30	Keynote speaker: Prof. Dr. André Studart (ETHZ)	*Evolving Bacteria to Make Materials*
	Student Presentations	
09:30 – 09:50	Hendrik Jansen	*Tailored Nanocrystalline Aluminium Grain Size in a Nanolaminated Architecture: New Horizons*
09:50 –10:10	Somashree Mondal	*Shape-morphing ferrimagnetic soft robots*
10:10 – 11:15	**First Poster Session (A) and Coffee**	
11:15 – 11:45	Keynote speaker: Prof. Dr. Anna Fontcuberta I Morral (EPFL)	*The joys and impact of research in materials science: a perspective from the semiconductor domain*
	Student Presentations	
11:45 – 12:05	Fabian Weyand	*Large-Scale Inkjet Printing of Graphene-Based Electrochemical Sensors*
12:05 – 12:25	Luis Mauricio Ortiz-Galvez	*Prospective material flow analysis and life cycle releases of graphene: enlightening a circular economy context for advanced materials in Europe*
12:25 – 13:30	**Lunch Break**	
13:30 – 13:50	Invited speaker: Natanael Lanz (Chiral Nano AG)	*How academic research led to Chiral Nano AG*
	Student Presentations	
13:50 – 14:10	Sandro Meier	*A first glimpse at the quantification of anthropogenic CH4 emissions in Europe with the Airborne Visible InfraRed Imaging Spectrometer AVIRIS-4*
14:10 – 14:30	Julia Achatz	*An Explainable Segmentation Decision Tree Model for Enhanced Decision Support in Roundwood Sorting*

14:30 – 14:50	Industry talk: Olivier Enger (BASF)	*A Journey towards Net Zero and Circularity*
	Student Presentations	
14:50 – 15:10	Marine de Lapeyrière	*Development of granular scaffolds from porous microgels for the treatment of skin burn wounds*
15:10 – 15:30	Kiarash Tajbakhsh	*Thyroid neoplasm pathology from micro anatomy to molecular signatures using X-ray imaging*
15:30 – 16:30	**Second Poster Session (B) and Coffee**	
16:30 – 16:50	Industry talk: Norbert Mayr (Metrohm)	*Research meets industry - A partnership for innovation*
	Student Presentations	
16:50 – 17:10	Hugo Braun	*Stable 4 V-class All-Solid-State Lithium Battery with Hydroborate Electrolyte and NMC811 Cathode*
17:10 – 17:30	Jiuke Chen	*Combined Computational and Experimental Study of Thermal Decomposition of Phosphorus Flame-retardants*
17:30 – 17:50	Industry talk: Raffael Kellner (VentureLab/ Venturekick)	*From science to startup: best practices on grants, venture capital, product launch, and scaling internationally*
17:50 – 18:30	Awards and Closing Ceremony	
18:30 – 19:00	**Apero**	
19:00 – 23:00	**Dinner (The Pavilion, Zürichstrasse 100, 8600 Dübendorf)**	

Speakers

Ms. Melina Spycher - Head Diversity and Inclusion Empa

Melina is a psychologist by training and current head of the Center of Competence for Diversity, Equity and Inclusion at PSI, Empa, and Eawag. Previously, she worked as behavioral psychologist, HR specialist, and deepened her knowledge regarding strategies and measures for a diverse, inclusive, and respectful work environment. If you want to contact her, connect with her on LinkedIn: https://www.linkedin.com/in/melinaspycher or via e-mail (melina.spycher@empa.ch).

Prof. Dr. André Studart, ETH Zürich

André Studart is Professor for Complex Materials at ETH Zurich, Switzerland. He obtained his BSc and PhD degrees in Materials Science and Engineering from the Federal University of São Carlos, Brazil. Before starting his group in Switzerland, he was postdoctoral researcher in the School of Engineering and Applied Sciences at Harvard University. The goal of his current research is to devise and study experimental platforms to create complex materials that replicate design principles of biological systems or harness the metabolic activity of microorganisms to generate unusual structures and properties. To achieve this goal, his research team works on bioinspired materials, printable materials, and living materials. In addition to academic research, Studart's group has also been active in technology transfer. This effort has led to spin-off companies in the areas of microencapsulation, additive manufacturing, and thermal management.

Prof. Dr. Anna Fontcuberta I Morral, EPF Lausanne

Professor Anna Fontcuberta i Morral has started her role as EPFL President as of January 1, 2025. She is a Full Professor in both Materials Science and Engineering and Physics and leads the Laboratory of Semiconductor Materials. Prior to her appointment, she served as the Associate Vice President for Centers and Platforms from 2021 until September 30, 2024.

She earned a bachelor's degree in physics from the University of Barcelona (Spain) in 1997 and went on to attain an impressive series of professional achievements. In 2001, she obtained a PhD in materials science from Ecole Polytechnique in Palaiseau (France). She served as a postdoc and a visiting scientist at the California Institute of Technology (USA) with Prof. Harry Atwater, with whom she co-founded Aonex Technologies. Before moving to Switzerland and joining EPFL in 2008, she worked as a team leader at the Technical University of Munich, where she obtained her habilitation in experimental physics.

Anna Fontcuberta i Morral has been a member of the Swiss National Science Foundation's Research Council since 2015. She served on its Presiding Board from 2020 to 2024 and acted among others as the president of the Specialized Committee for International cooperation. She is furthermore member of the EPFL-WISH foundation and its former president, a foundation whose goal is to support female students in accomplishing their professional goals. She is also a member of the Swiss Quantum Commission of the Swiss Academy of Science.

Among the awards she has received are the Marie Curie Excellence Grant, ERC Starting Grant, the SNSF-backup schemes Consolidator Grant, and the European Physical Society Emy Noether prize.

Natanael Lanz, Chiral Nano AG

Natanael Lanz did his Bachelor's and master's studies at ETH in Mechanical Engineering. Thereafter, he did his PhD in the institute for machine tools and manufacturing (IWF, ETH) under the supervision of Prof. Dr. Konrad Wegener, with a focus on optimizing mechatronic motion systems by measurement and control improvements. Part of it was, the project that led to Chiral. Next, he was a Pioneer Fellow in the micro- and nano-systems lab under the supervision of Prof. Christofer Hierold. The spinning-out of Chiral as a private company was the result of the program. Today he is the CTO at Chiral since, responsible for developing our technology to reach product market fit.

Olivier Enger, BASF

Olivier Enger is a Senior Principal Scientist / Technology Scout in the central R&D division of BASF. He studied at the university of Strasbourg (F) and Cambridge (UK) before getting is Ph.D. from the ETH Zürich with Prof. F. Diederich in 2002. After a postdoctoral stay with Prof. Dr. F. Stoddart at UCLA (USA), Olivier started his career at BASF SE (DE) in 2003 as Research team leader in the field of liquid crystals and organic electronics. Moving from team leader to marketing manager for active pharmaceutical ingredients and then global R&D group leader for photo initiators and special dyes, he is now a technology scout at BASF Switzerland since 2012. He is co-located at the Empa in Dübendorf for close collaboration and co-creation with the Empa and the NEST (in which BASF and partners have set up the new unit "STEP2"), and more broadly the ETH innovation ecosystem. Although his focus if broadly on sustainable technologies, he is more specifically interested in net zero technologies, sustainable materials and digital construction.

Norbert Mayr, Metrohm

Dr. Norbert Mayr received his diploma in chemistry from the University of Ulm and his Ph.D. from the Ludwig-Maximilan-University in Munich.

His studies span a wide range of material science, from crystallization processes for bio-inorganic research to high energy dense materials and inorganic molecule chemistry.

The career outside of university followed the stations of account management, product training and product management.

The recent position at Metrohm AG in Switzerland is Head of Competence Center Innovation and Digitalization.

Raffael Kellner, VentureLab/ Venture-kick

Raffael Kellner supports spin-offs from Swiss universities, getting them ready for grants, venture capital, product launch, and scaling internationally. He is the lead organizer of startup investor roadshows to China, India, and UK, as well as of the Venture Challenge at ETH, the PSI Entrepreneurship Course, and the Venture Briefing program hosted at Swiss research institutions. Raffael also personally invests in Swiss startups through the Kick Fund. Prior to Venturelab / Venture Kick, Raffael has been a co-founder of two startups and worked in corporate advisory positions in Zurich, New York, Hong Kong, Vienna, Bratislava, and Berlin.

Student Presentations

Hendrik Jansen - Empa, Mechanics of Materials and Nanostructures

Tailored Nanocrystalline Aluminium Grain Size in a Nanolaminated Architecture: New Horizons

Hendrik C Jansen[a,b], Amit Sharma[a,c] , Barbara Putz[a], Marcus Hans[d], Jochen M Schneider[d], Jakob Schwiedrzik[a,e], Thomas EJ Edwards[a,f] , and Johann Michler[a,b]

[a] *Laboratory for Mechanics of Materials and Nanostructures, Empa Swiss Federal Laboratories for Material Science and Technology, Feuerwerkerstrasse 39, CH-3602 Thun, Switzerland*

[b] *École Polytechnique Fédérale de Lausanne, Rte Cantonale, CH-1015 Lausanne, Switzerland*

[c] *SwissCluster AG, Bahnhofstrasse 19, CH-3700 Spiez, Switzerland*

[d] *Materials Chemistry, RWTH Aachen University, Kopernikusstrasse 10, D-52074 Aachen, Germany*

[e] *Laboratory for High Performance Ceramics, Empa Swiss Federal Laboratories for Material Science and Technology, Überlandstrasse 129, CH-8600 Dübendorf, Switzerland*

[f] *Research Center for Structural Materials, National Institute for Materials Science, 1-2-1 Sengen, J305-0047, Japan*

Key Words: Nanocrystalline Aluminium, Hybrid multilayer thin film deposition, Micromechanics

INTRODUCTION: Grain growth limits the applicability of engineering metals alike Aluminium (Al) alloys. Coarse-grained Al microstructures usually result in reduced mechanical properties – risking catastrophic failure [1,2]. In this work, we are reporting interface-engineered AlNi - AlOH (25 – 1 nm) thin films with tailored impediment of Al grain growth in two dimensions - expanding the application of engineering Al alloys.

METHODS: The thin films were deposited by means of combined hybrid physical vapour (PVD) and atomic layer deposition (ALD) in a SwissCluster AG SC-1 cluster deposition chamber. Mechanical testing was conducted by Nanoindentation with a Berkovich tip. High-resolution analysis of the microstructure was performed by means of combined transmission electron microscopy and atom probe tomography.

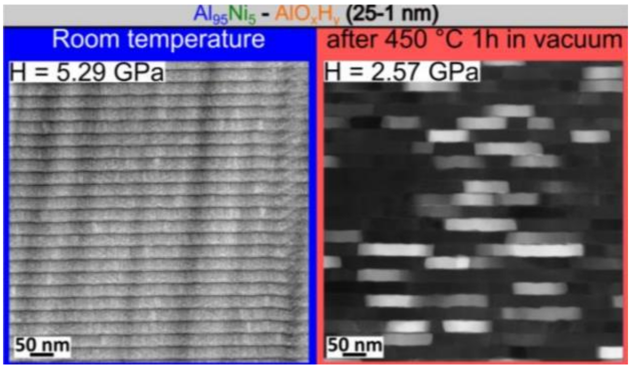


Fig. 1: Scanning transmission electron microscopy image of $Al_{95}Ni_5$ – AlOH at room temperature and after vacuum annealing at 450 °C for 1 h with insets of nanoindentation hardness.

RESULTS & DISCUSSION: As-deposited $Al_{95}Ni_5$ – AlOH (25 – 1 nm) thin films are reported to possess a lateral FCC Al grain size of only 10 nm with fine 1 nm Ni-rich segregations and roughly 1 nm AlOH interlayers. This unique microstructure is set to explain the > 5 GPa Nanoindentation hardness of the thin film stack. Vacuum annealing at various temperatures is gradually lowering the hardness until reaching 2.6 GPa for vacuum annealing at 450°C for 1 h, where interlayers set to broaden and Al-Ni phase separation completes.

CONCLUSIONS: AlNi - -AlOH (25 – 1 nm) thin films with > 5 GPa as-deposited hardness show superior mechanical response, even at elevated temperatures. Thus, the system serves asblueprint for further developing Al-based engineering materials towards higher strength and thermal stability with novel combination of deformation mechanisms.

ACKNOWLEDGEMENTS: HCJ acknowledges Innosuisse Innovation project 109.352.1 "ORALCOAT" as well as ScopeM for support and assistance in this work.

REFERENCES:

[1] Q. Li, J. Wang, H. Wang, X. Zhang, Achieving strong and stable nanocrystalline Al alloys through compositional design, J. Mater. Res. 37 (2022) 183–207.

[2] Z. Chen, F. Liu, H.F. Wang, W. Yang, G.C. Yang, Y.H. Zhou, A thermokinetic description for grain growth in nanocrystalline materials, Acta Mater. 57 (2009) 1466 – 1475

Somashree Mondal – Empa, High Performance Ceramics

Shape-morphing ferrimagnetic soft robots

Somashree Mondal[1,2], Ralph Spolenak[2], Frank Clemens[1]

[1] *Laboratory of High Performance Ceramics, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Laboratory of Nanometallurgy, ETH Zürich, Zürich, Switzerland*

Keywords: Magnetic soft robots, small-scale robots, additive manufacturing, magnetoactive soft elastomers

Graphical abstract

Magnetic soft robots are well-known for their compliance, untethered nature and controllability. From drug or cargo delivery to minimally invasive surgery, they are a promising candidate for a range of applications. However, the most commonly investigated material for such soft robots is neodymium iron boron (NdFeB) comprising composites [1], [2]. Although NdFeB exhibits commendable magnetic properties, a high magnetic field (> 2 T) is required to permanently magnetize it [3]. In this work, we have developed millimeter-scaled magnetic soft robots using additive manufacturing of magnetoactive soft elastomers comprising strontium hexaferrite ($SrFe_{12}O_{19}$) particles since they can be magnetized at lower fields (~ 1 T). To actuate the soft robots, we applied magnetic fields in distinct ways to program the hard ferrimagnetic domains. To investigate the shape-morphing characteristics of the milli-robots we used a custom test setup equipped with a microcontroller, electromagnet and a laser distance sensor [4]. We used simple rectangular geometry to investigate different aspects like the optimum magnetic field required for magnetization, bending angle, radius of curvature and magnetic flux distribution in the programmed robot. With increasing magnetic field produced by the electromagnet (14 to 51 mT), the bending of the rectangular robot increased and the radius of curvature decreased almost by two times

Furthermore, we investigated other magnetic soft robots performing actions like lifting, flapping and passive-crawling. Here we introduce a time- and cost-efficient approach to developing ferrimagnetic milli-robots. This opens new avenues for cost-effective applications of small-scaled magnetic soft robots.

REFERENCES:

[1] W. Hu, G. Z. Lum, M. Mastrangeli, and M. Sitti, "Small-scale soft-bodied robot with multimodal locomotion," Nature, vol. 554, no. 7690, Art. no. 7690, Feb. 2018, doi: 10.1038/nature25443.

[2] T. Xu, J. Zhang, M. Salehizadeh, O. Onaizah, and E. Diller, "Millimeter-scale flexible robots with programmable three-dimensional magnetization and motions," Sci. Robot., vol. 4, no. 29, p. eaav4494, Apr. 2019, doi: 10.1126/scirobotics.aav4494.

[3] Y. Kim, G. A. Parada, S. Liu, and X. Zhao, "Ferromagnetic soft continuum robots," Sci. Robot., vol. 4, no. 33, p. eaax7329, Aug. 2019, doi: 10.1126/scirobotics.aax7329.

[4] P. Orkisz, S. Mondal, F. Clemens, T. Graule, and B. Sapiński, "Expanding the Research Capabilities of an Experimental Setup for Testing Magnetoactive Materials," in 2024 25th International Carpathian Control Conference (ICCC), May 2024, pp. 1–5. doi: 10.1109/ICCC62069.2024.10569720.

Fabian Weyand - Empa, Nano Particles

Large-Scale Inkjet Printing of Graphene-Based Electrochemical Sensors

Fabian Weyand[a]

[a]*Department 500 – Energy, Mobility and Environment*

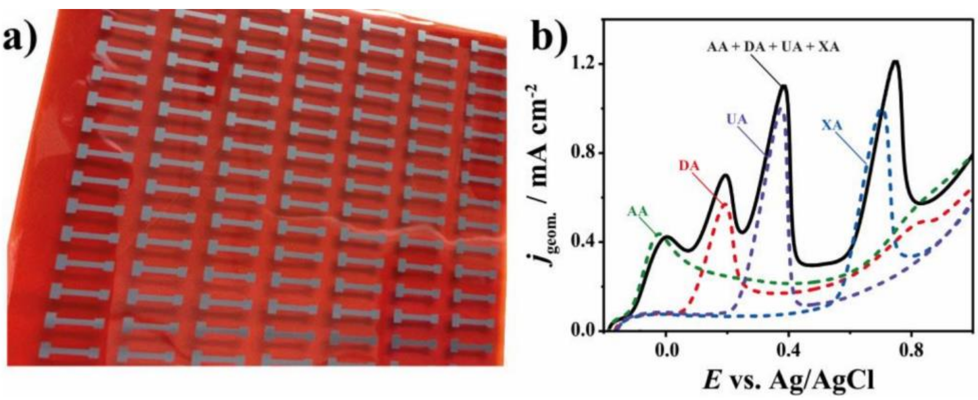


Fig.1: Large-scale production of inkjet-printed graphene electrodes (**a**). Sensitive and selective voltammetric detection of UA in the presence of ascorbic acid (AA), dopamine (DA) and Xanthine (XA) (**b**).

The global demand for disposable, electrochemical sensors for the detection of biomolecules has driven the development of large-scale, screen-printing-based manufacturing techniques for decades, e.g., a deciding factor for the success of electrochemical blood glucose sensing.[1] However, screen printing of high-performance sensing materials such as graphene can be costly as a large portion of the material is lost as ink residue on the screen, while modifying the sensor design requires physical changes to the screen, which limits process automation. Therefore, digital and mask-less drop-ondemand inkjet printing, using ejection of picolitre-sized droplets at kHz frequencies enables process automation with ideally zero material waste in a reasonably short time, although the absence of a mask can cause sensor-to-sensor variations through lower printing resolution.[2]

In this presentation, we will introduce graphene electrodes, fabricated on large-scale using inkjet printing with highly optimized parameters (**Fig. 1**). Defined post-print heat treatments result electrodes that provide reproducible voltammetric sensing signals for the detection of benchmark biomolecules (e.g., uric acid (UA)) and their adsorption-driven enhanced sensitivities and selectivity outperform state-of-the-art carbon materials like glassy carbon. Heating under vacuum and air, respectively, suppresses and enhances adsorption-boosted sensitivities in a repetitive manner, enabling interesting opportunities for applications where non-specific adsorption is detrimental.Inkjet printing along with distinct heating protocols has great potential to produce reproducible and cost-effective sensors with the option of upscaling the fabrication process from prototype level to industrial scales.

Future benefit for society: The optimization of inkjet printing processes for the large-scale production of high-performance biomolecular sensors not only has great potential to outperform previous manufacturing processes, but also to make the global demand for flexible and disposable sensors for medically relevant point-of-care detection no longer a question of money.

[1] Abellán-Llobregat, A., et al., Biosens. Bioelectron. **2017**, 91, 885-891.

[2] Nagar, B., et al., ChemElectroChem **2020**, 7(2), 460-468

Luis Mauricio Ortiz-Galvez - Empa, Technology and Society

Prospective material flow analysis and life cycle releases of graphene: enlightening a circular economy context for advanced materials in Europe

Luis Mauricio Ortiz-Galvez[1], Lora Dameska[1,2] and Bernd Nowack[1]

[1] Empa, Technology & Society Laboratory, 9014 St. Gallen, Switzerland;

[2] Chemical Engineering Department, Université de Liège, Quartier Agora, B6A 11, Allée du 6 Août, 4000 Liege (Sart Tilman), Belgium.

INTRODUCTION: Advanced materials (AdMas) are found in multiple industrial sectors. Nevertheless, their environmental safety evaluation remains challenging, mainly during the End-of-life and recycling processes, which is relevant in the transition towards a circular economy (CE).

METHODS: This study employed Dynamic Probabilistic Material Flow Analysis and prospective scenarios (waste-as-usual (S1), EU waste-policy targets (S2), and circular economy (S3) scenarios) to evaluate potential flows of graphene in tires, batteries, and concrete (TBC system), in Europe from 2025 to 2050, based on [1].

RESULTS & DISCUSSION: Simulating the TBC system, the amount of graphene mass flowing and released depends on each scenario. However, once graphene is released, more than 90% of the environmental releases of graphene, coming from production and manufacturing, go mainly to soil, regardless of the scenario. However, assuming a CE context (S3), there is a decrease in improper disposal and export. Thus, most of the mass goes into elimination, then to reuse, recycling, and recycling residues, that might then go into concrete (Fig. 1) because of the use of residues as backfillers.

CONCLUSIONS: This study assessed prospective flows and releases of graphene in the TBC system in Europe. According to the model, graphene flows predominantly exit the system or accumulate in technical compartments, with concrete emerging as a sink for (persistent) AdMas, which should be further investigated and included in CE scenarios. This research showed that MFA is useful for exploring industrial symbiosis and CE strategies and evaluating if products could unintentionally contain AdMas in circular life cycles.

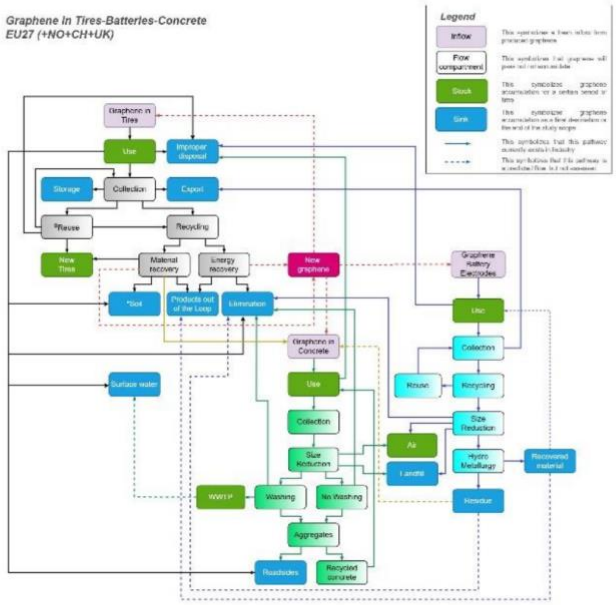


Fig. 1: Current and prospective flows of graphene in the Tires-Batteries-Concrete system in Europe. WWTP stands for Wastewater treatment plants; *Soil refers to multiple applications on soil and direct releases; and αReuse refers to direct reuse, retreading, and regrooving of tires

ACKNOWLEDGEMENTS: MACRAMÉ project with grant agreement number – 101092686 and State Secretariat for Education, Research and Innovation (SERI) no 23.0014

DECLARATION OF THE USAGE OF AI: ChatGPT was used to summarize the original abstract to a maximum of 250 words.

REFERENCES:

[1] Hong et al., Environ. Sci. Technol. (2022). 56, 19, 13798–13809

Sandro Meier - Empa, Air Pollution / Environmental Technology

A first glimpse at the quantification of anthropogenic CH4 emissions in Europe with the Airborne Visible InfraRed Imaging Spectrometer AVIRIS-4

Sandro Meier[1,2], Marius Vögtli[2], Andreas Hüni[2], Dominik Brunner[1], Gerrit Kuhlmann[1]

[1]*Empa, Laboratory for Air Pollution/Environmental Technology, Ueberlandstrasse 129,*

8600 Duebendorf, Switzerland (sandro.meier@empa.ch)

[2]*Remote Sensing Laboratories, Department of Geography, University of Zurich, Winterthurerstrasse 190, 8057 Zurich, Switzerland*

Fig. 1: Example of a detected CH_4 plume from the controlled release experiment in France.

INTRODUCTION: Methane (CH_4), a potent greenhouse gas with a global warming potential 28 times higher than CO_2, has seen its atmospheric concentration rise due to natural and anthropogenic sources such as agriculture, fossil fuels, and waste. With a short atmospheric lifetime of nine years, reducing CH_4 emissions is a key strategy to mitigate climate change. However, significant uncertainties remain in quantifying anthropogenic emissions. Remotely sensed observations, using a top-down approach, offer a means to address these uncertainties (Saunois et al. 2020).

METHODS: A state-of-the-art high-resolution sensor capable of detecting CH_4 is the new Airborne Visible InfraRed Imaging Spectrometer AVIRIS-4 (Shaw et al. 2022). During summer and autumn 2024, we conducted flight campaigns focusing on landfills, compressor stations, and coal mines across Italy, France and Germany where we acquired over 160 flight lines at various altitudes. To exploit the capabilities of AVIRIS-4 for CH_4 retrieval, we implemented a matched filter to retrieve the CH_4 column concentrations from hyperspectral imagery (Foote et al., 2020). We estimate the emissions using the Integrated Mass Enhancement (IME) method, which we validated based on simulations from the state-of-the-art MicroHH model (Kuhlmann et al., 2024).

RESULTS & DISCUSSION: Our preliminary analysis shows that AVIRIS-4 can detect CH_4 at a spatial resolution of 30 - 50 cm, which allows for the differentiation of spatially proximate plumes. The initial findings suggest that AVIRIS-4 can be employed to estimate emissions exceeding 10 kg/h.

CONCLUSIONS: Our first results highlight the potential of AVIRIS-4 to advance CH_4 emission quantification and mitigation efforts.

ACKNOWLEDGEMENTS: This research has been funded under the framework of UNEP's International Methane Emissions Observatory (IMEO).

REFERENCES:

Foote, M.D., Dennison, P.E., Thorpe, A.K., Thompson, D.R., Jongaramrungruang, S., Frankenberg, C., & Joshi, S.C. (2020). Fast and Accurate Retrieval of Methane Concentration From Imaging Spectrometer Data Using Sparsity Prior. IEEE Transactions on Geoscience and Remote Sensing, 58, 6480-6492

Kuhlmann, G., Koene, E.F.M., Meier, S., Santaren, D., Broquet, G., Chevallier, F., Hakkarainen, J., Nurmela, J., Amorós, L., Tamminen, J., & Brunner, D. (2024). The ddeq Python library for point source quantification from remote sensing images (Version 1.0)

Saunois, M., Stavert, A.R., Poulter, B., Bousquet, P., Canadell, J.G., Jackson, R.B., Raymond, P.A., Dlugokencky, E.J., Houweling, S., Patra, P.K., Ciais, P., Arora, V.K., Bastviken, D., Bergamaschi, P., Blake, D.R., Brailsford, G., Bruhwiler, L., Carlson, K.M., Carrol, M., Castaldi, S., Chandra, N., Crevoisier, C., Crill, P.M., Covey, K., Curry, C.L., Etiope, G., Frankenberg, C., Gedney, N., Hegglin, M.I., Höglund-Isaksson, L., Hugelius, G., Ishizawa, M., Ito, A., Janssens-Maenhout, G., Jensen, K.M., Joos, F., Kleinen, T., Krummel, P.B., Langenfelds, R.L., Laruelle, G.G., Liu, L., Machida, T., Maksyutov, S., McDonald, K.C., McNorton, J., Miller, P.A., Melton, J.R., Morino, I., Müller, J., Murguia-Flores, F., Naik, V., Niwa, Y., Noce, S., O'Doherty, S., Parker, R.J., Peng, C., Peng, S., Peters, G.P., Prigent, C., Prinn, R., Ramonet, M., Regnier, P., Riley, W.J., Rosentreter, J.A., Segers, A., Simpson, I.J., Shi, H., Smith, S.J., Steele, L.P., Thornton, B.F., Tian, H., Tohjima, Y., Tubiello, F.N., Tsuruta, A., Viovy, N., Voulgarakis, A., Weber, T.S., Van Weele, M., Van Der Werf, G.R., Weiss, R.F., Worthy, D., Wunch, D., Yin, Y., Yoshida, Y., Zhang, W., Zhang, Z., Zhao, Y., Zheng, B., Zhu, Q., Zhu, Q., & Zhuang, Q. (2020). The Global Methane Budget 2000–2017. Earth System Science Data, 12, 1561-1623

Shaw, L.A., Geier, S., Mckinley, I.M., Bernas, M.A., Gharakhanian, M., Dergevorkian, A., Eastwood, M.L., Mouroulis, P., Green, R.O., 2022. Design, alignment, and laboratory calibration of the Compact Wide Swath Imaging Spectrometer II (CWIS-II). Imaging Spectrom. XXV: Appl., Sens., Process. 12235, 1223502-1223502–10. https://doi.org/10.1117/12.2634282

An Explainable Segmentation Decision Tree Model for Enhanced Decision Support in Roundwood Sorting

Julia Achatz[1*], Pauline Sailer[2], Sven Mayer[2], Mark Schubert[1*]

[1] *Cellulose and Wood Materials, Group WoodTec, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Media Informatics Group, LMU Munich, München, Deutschland*

INTRODUCTION: Recent industry insights revealed an urgent need for affordable automation and Decision Support Systems (DSSs) in grading roundwood. Such systems are essential for fair pricing, efficient and objective sorting, and optimal resource utilization. Transparency and explainability are crucial for industry adoption, as they maintain integrity with trade customs, facilitate model improvements, build user trust, and aid in training new employees.

METHODS: To address this need, we introduce the Segmentation Decision Tree (SegDT) classifier, a hybrid-interpretable method that combines image segmentation for feature extraction with a decision tree for quality classification. To provide context, we investigate state-of-the-art Explainable Artificial Intelligence (XAI) methods, including Gradient-weighted Class Activation Mapping (GradCam), to address the black-box nature of Convolutional Neural Networks (CNNs) in industrial roundwood sorting. Further we compare the CNN + GradCam model and the SegDT classifier, focusing on accuracy and explainability. A quantitative user study assessed both systems, emphasizing user experience and trust.

RESULTS & DISCUSSION: The SegDT classifier achieved an accuracy of 80% in distinguishing between three main quality grades, matching the performance of CNN-based models. However, the study indicated a clear preference for the SegDT over the CNN + GradCam prototype.

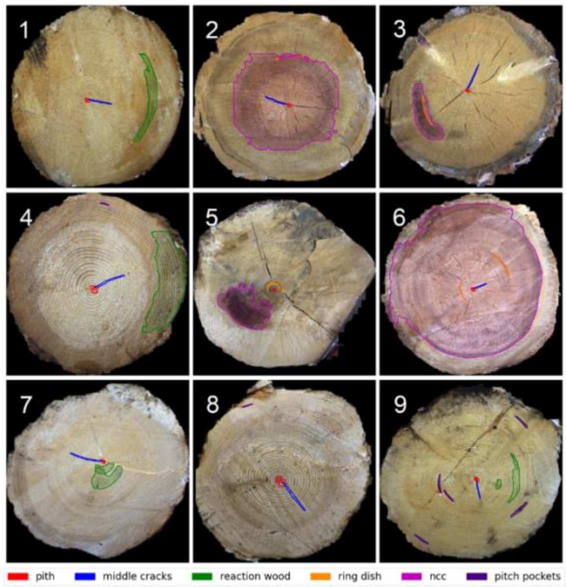


Fig. 1: *Example of cross-sectional images with different features detected by a YOLOv8x instance segmentation model.*

CONCLUSIONS: While both systems demonstrate the potential to improve efficiency and accuracy, the SegDT system stands out for its transparency and usability, making it a highly suitable solution for the industry. For a video summary of this paper, please visit https://youtu.be/A1w1rYWOWxo.

ACKNOWLEDGEMENTS: We express our sincere gratitude to Mr. Thomas Lädrach and Mrs. Nathalie Lädrach of our industry partner OLWO AG for their support throughout the project. We also extend our thanks to Mr. Erich Salzmann from OLWO AG for sharing his expertise in roundwood inspection.

Marine de Lapeyrière - Empa, Biointerfaces

Development of granular scaffolds from porous microgels for the treatment of skin burn wounds

Marine de Lapeyrière[1], Martina Viola[1], Fabian Itel[2], Katharina Maniura[1], Markus Rottmar[1]

[1]Biointerfaces laboratory, [2] Laboratory for Biomimetic Membranes and Textiles, Empa, Swiss Federal Laboratories for Materials Science and Technology, Switzerland Sankt Gallen

INTRODUCTION: Healing of skin burn wounds is a complex process and depends, among other things, on cell infiltration into and deposition of extracellular matrix (ECM) in the wound site. Hydrogels are very promising materials to promote healing of skin burn wounds, but depending on their properties, cell infiltration and handling of excessive amounts of exudate can be limited by bulk hydrogels. Granular hydrogels have offered great promise to address these challenges, but controlling their porosity is of key importance for cell infiltration, ECM deposition and wound fluid transport.

The goal of this project is the rapid fabrication of granular microgel 3D scaffolds and to explore their potential use for the treatment of skin burn wounds. To this end, scaffold designs originating from the combination of differently sized porous microgels are explored for their mechanical properties and their void space distribution/porosity to enhance cell infiltration as well as ECM deposition.

METHODS: Blended polymer microgels are fabricated by aerodynamically assisted jetting a solution of alginate and norbornene-PVA (nPVA)[1] into a $CaCl_2$ bath to achieve rapid gelation of alginate. Mixing in a photoinitiator (i.e. LAP) and a di-thiolated crosslinker (i.e. DTT, PEG dithiol or an MMP-sensitive peptide) allows for subsequent photo-crosslinking of nPVA. To obtain porous microgels, alginate is then removed from the microgels by incubating them in alginate lyase. Macrogels are subsequently fabricated by binding microgels together via photo-crosslinking by soaking the nPVA microgels in a photoinitiator/crosslinker solution and subsequent exposure to UV.

RESULTS: Rapid fabrication of large amounts of alginate/nPVA microgels could be achieved by aerodynamically assisted jetting (approx. 0.3M beads from 1ml of precursor solution). The resulting beads show a spherical shape with sizes ranging from ~20 to ~70 µm. Specific size fractions could afterwards be obtained by the sequential use of differently sized filters.

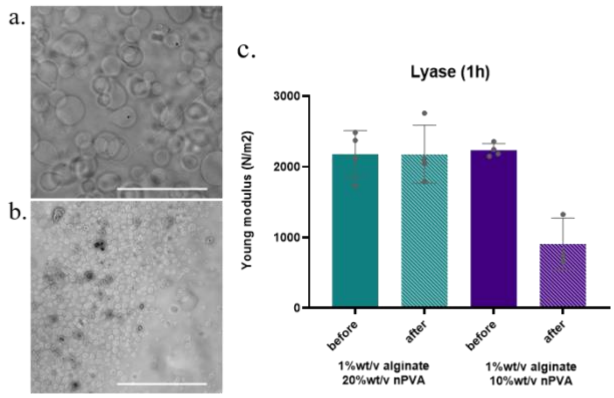


Figure: Brightfield images of alginate/nPVA microgels a. right after fabrication and b. after 24h incubation in a solution of 0.5mg/ml of alginate lyase (scale bar: 100µm). c. Young Modulus from compression tests (compression up to 50% of scaffold original height) on alginate/nPVA hydrogels before and after being incubated in a solution of 1mg/ml alginate lyase for 1h.

The obtained microgels conserved their shape when kept in a $CaCl_2$-containing solution, facilitating subsequent crosslinking of the nPVA by UV light. Once collected, the alginate in the microgels was degraded by incubation in an alginate lyase solution, leading to a both smaller and softer material.

DISCUSSION & CONCLUSIONS: Aerodynamically assisted jetting is a promising approach for the rapid fabrication of large numbers of alginate/nPVA microgels. The obtained beads show excellent shape fidelity and narrow size distribution. Alginate can be removed from alginate/nPVA, thus offering great promise to form porous microgels. Macroporous granular hydrogels will in future be assessed for mechanical properties, fluid transport, cell infiltration and ECM deposition.

REFERENCES:

1. Qin, X.H., et al., Adv Mater, 2018. **30**(10).

Kiarash Tajbakhsh – Empa, Center for X-ray Analytics

Thyroid neoplasm pathology from micro anatomy to molecular signatures using X-ray imaging

Kiarash Tajbakhsh[1], Jonas Bossart[2], Olga Stanowska[3*], Marija Bulja[2], Aurel Perren[3], Antonia Neels[1], Robert Zboray[1].

[1] *Center for X-ray Analytics, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Nanomaterials in Health, Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, Switzerland*

[3] *Institute for tissue medicine and pathology, University of Bern, Bern, Switzerland.*

INTRODUCTION: The diagnosis of thyroid neoplasms relies on 2D histology, limited by sampling bias and artifacts [1], which compromises accuracy. X-ray phase contrast imaging (XPCI) enables non-destructive 3D imaging of pathological specimens with exceptional resolution and contrast [2]. Combining deep learning and texture analysis [3], imaging-based biomarkers can be extracted from 3D images relating to molecular alterations, providing a standalone comprehensive diagnostic and prognostic tool that provides diagnostics based on traditional standards [4], as well as emerging molecular finger prints [5].

METHODS: FFPE blocks were imaged with XPCI, and a deep learning model is trained for segmentation. Histological validation was used to confirm XPCI findings. Texture analysis using mathematical modeling, as well as deep learning is used for molecular finger prints classification.

RESULTS & DISCUSSION: XPCI enabled detection of capsular and vascular invasions, key factors in classifying follicular thyroid carcinoma (FTC) [6]. This result motivated a collaboration across Austria, Germany, and Switzerland to investigate relapse cases, revealing pathologies missed due to sampling bias. A deep learning segmentation model is being trained to reduce subjectivity in diagnosis.

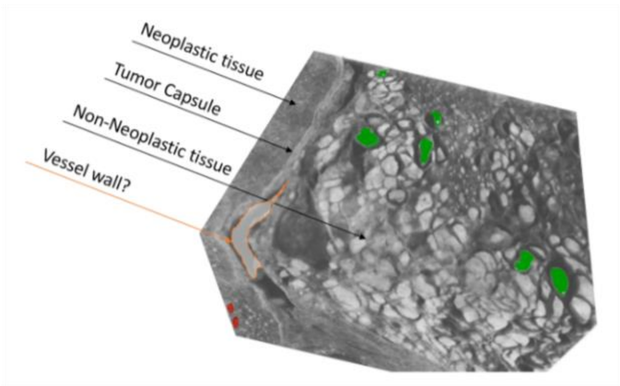


Fig. 1: XPCI of a FTC. Showing neoplastic, non-neoplastic, and capsule wall. Demonstrating XPCI ability to visualize micro anatomy of FTCs.

Based on texture analysis, a classification model was developed, achieving AUROC scores of 0.93±0.01 (tumor vs. healthy), 0.85±0.01 (PTC vs. FTC), 0.84±0.04 (BRAF V600E mutation), and 0.83±0.03 (relapse prediction).

CONCLUSIONS: This project demonstrates the potential of XPCI and deep learning to revolutionize digital pathology by enabling 3D imaging, accurate segmentation, and surrogate imaging biomarkers for molecular alterations. XPCI can be a standalone diagnostic and prognostic tool, addressing limitations of traditional 2D histology and facilitating personalized medicine.

ACKNOWLEDGEMENTS: This work was supported by the Strategic Focus Area Personalized Health and Related Technologies (PHRT) of the ETH-Domain, PHRT Pioneer Imaging Project under Grant 2021-614.

REFERENCES:

[1] Taqi, Syed Ahmed, et al. "A review of artifacts in histopathology." *Journal of oral and maxillofacial pathology* 22.2 (2018): 279.

[2] Tajbakhsh, Kiarash, et al. "A comprehensive study of laboratory-based micro-CT for 3D virtual histology of human FFPE tissue blocks." *IEEE Access* (2024).

[3] Miotto, Riccardo, et al. "Deep learning for healthcare: review, opportunities and challenges." *Briefings in bioinformatics* 19.6 (2018): 1236-1246.

[4] G. Tallini et al., "Thyroid gland" in Endocrine and Neuroendocrine Tumours, Lyon, France:IARC, 2022.

[5] Bossart, Jonas, et al. "Mapping the Molecular Landscape of Thyroid Neoplasms: A Comprehensive Proteomic and Phosphoproteomic Analysis Across Tumors of Follicular Origin." *bioRxiv* (2024): 2024-11.

[6] Tajbakhsh, Kiarash, et al. "3D virtual histopathology by phase-contrast X-ray micro-CT for follicular thyroid neoplasms." *IEEE Transactions on Medical Imaging* (2024).

Hugo Braun - Empa, Materials for Energy Conversion

Stable 4 V-class All-Solid-State Lithium Battery with Hydroborate Electrolyte and NMC811 Cathode

Hugo Braun[1,2], Ryo Asakura[1], Arndt Remhof[1,2], Corsin Battaglia[1,3,4]

[1] *Empa – Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Institut für Anorganische und Analytische Chemie, Albert-Ludwigs-Universität Freiburg, Germany*

[3] *Department of Information Technology and Electrical Engineering, ETH Zurich, Switzerland*

[4] *School of Engineering, Institute of Materials, EPFL, Switzerland*

Solid-state batteries are expected to extend the energy and power density beyond the limits of today's lithium-ion batteries, and to replace their flammable liquid electrolyte with safer alternatives. To date, there are only few solid electrolytes fulfilling simultaneously the high demands in terms of ionic conductivity, chemical and electrochemical stability, and mechanical properties. Hydroborates combine many attractive characteristics such as high ionic conductivity, compatibility with alkali metal anodes and soft mechanical properties, but are challenging to integrate into batteries with high-voltage cathodes.

Here, we demonstrate stable dis-/charge cycling of solid-state lithium-ion batteries combining a $Li_3(CB_{11}H_{12})_2(CB_9H_{10})$ hydroborate electrolyte with a 4 V-class $LiNi_{0.8}Mn_{0.1}Co_{0.1}O_2$ (NMC811) cathode,

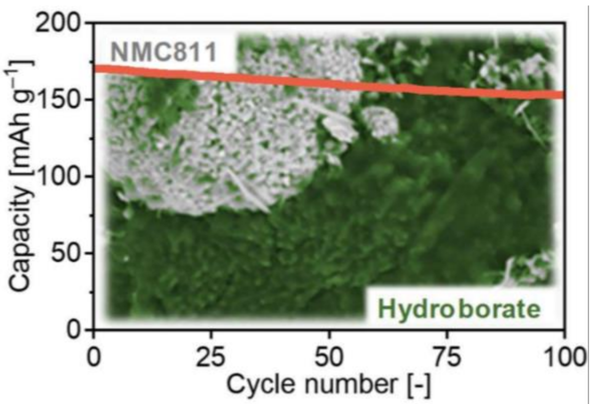


Fig. 1: *Discharge capacity over 100 cycles of the solid-state hydroborate battery at 60 °C, and SEM image of the NMC811 particles (grey) embedded in* $Li_3(CB_{11}H_{12})_2(CB_9H_{10})$ *electrolyte*

(green).[1]

exploiting the enhanced kinetic stability of the $LiCB_{11}H_{12}$-rich and $LiCB_9H_{10}$-poor electrolyte composition.[1] Cells with lithium metal and indium/lithium anodes achieve a discharge capacity at C/10 of ~145 mAh g^{-1} at room temperature and ~175 mAh g^{-1} at 60 °C (Figure 1). Indium/lithium cells retain 98% of their initial discharge capacity after 100 cycles at C/5 (room temperature) and 70% after 1000 cycles at C/2 (60 °C). Capacity retention of 97% after 100 cycles at C/5 and 75% after 350 cycles at C/2 is also achieved with a graphite anode without any excess lithium.

The energy density per cathode composite weight of 460 Wh kg^{-1} is on par with the best solid-state batteries reported to date, demonstrating the potential of hydroborate electrolytes to deliver a competitive next-generation battery technology.

REFERENCES:

[1] Braun, H.; Asakura, R.; Remhof, A.; Battaglia, C. ACS Energy Lett. 2024, 9 (2), 707-714.

Jiuke Chen – Empa, Advanced Fibers

Combined Computational and Experimental Study of Thermal Decomposition of Phosphorus Flame-retardants

Jiuke Chen[1,2], Sabyasachi Gaan[1], Sin Yong[3], Sandro Lehner[1], Daniele Passerone[4], Manfred Heuberger[1,2,*], Ali Gooneie[3]

[1] Laboratory of Advanced Fibers, Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, Switzerland

[2] ETH Zurich, Department of Materials, Switzerland

[3] Circular Plastics, Department of Circular Chemical Engineering, Faculty of Science and Engineering, Maastricht University, Urmonderbaan 22, 6162 AL Geleen, The Netherlands

[4] Nanotech@surfaces Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, Überlandstrasse 129, Dübendorf, 8600 Switzerland

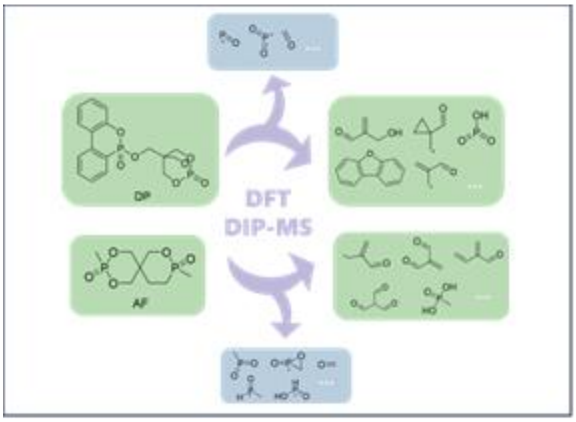


Fig. 1: The decomposed products of DP and AF.

INTRODUCTION: Phosphorus flame retardants (P-FRs) have gained significant attention as crucial and environmentally preferable additives in various applications, thanks to their superior FR properties and lower toxicity compared to traditional halogenated FRs[1]. With the increasing production and use of P-FRs, it becomes essential to understand their sustainability and recyclability. A key aspect involves studying the interactions between P-FRs and polymeric matrices [2–4]. To address this, we employed a combination of computational and experimental techniques to investigate the thermal decomposition of two specific P-FRs, DOPO-PEPA (DP) and Aflammit PCO 900 (AF).

METHODS: The density functional theory (DFT) calculations were coupled with the direct insertion probe mass spectrometry (DIP-MS) and a series algorithm for data processing.

RESULTS & DISCUSSION: Two major decomposition pathways were investigated, starting with proton attack and bond dissociation. The potential decomposed products, especially the phosphorus-containing species acting in the gas phase, were confirmed by the combination of DFT and DIP-MS spectra. In addition, the transition state theory was used to obtain the potential energy surfaces along the decomposition pathways and then to acquire the rate constants.

CONCLUSIONS: Our findings detailed how DP and AF, two of the most significant P-FRs, break down into phosphorus-containing species and other potential species that may interact with the polymer matrix. This research not only deepens our understanding of P-FR behavior during the mechanical recycling but also lays the groundwork for developing sustainable and recyclable P-FR solutions.

ACKNOWLEDGEMENTS: We acknowledge the financial support by Empa for the "ReFR" project. We appreciate Dr. Arvindh Sekar, Dr. Cédric Hervieu, Dr. Rudolf Hufenus, and Dr. Wenyu Wu Klingler for their advice and support.

REFERENCES:

[1] A. Bifulco, C. Varganici, L. Rosu, F. Mustata, D. Rosu, S. Gaan, Polymer Degradation and Stability 200 (2022) 109962.

[2] J. Chen, S. Dul, S. Lehner, M. Jovic, S. Gaan, M. Heuberger, R. Hufenus, A. Gooneie, Journal of Materials Science & Technology (2024).

[3] C. Bascucci, I. Duretek, S. Lehner, C. Holzer, S. Gaan, R. Hufenus, A. Gooneie, Polymer Degradation and Stability 195 (2022) 109783.

[4] A. Gooneie, P. Simonetti, P. Rupper, R. Nazir, M. Jovic, S. Gaan, M.P. Heuberger, R. Hufenus, Materials Letters 276 (2020) 128225.

[5] F. Neese, WIREs Computational Molecular Science 12 (2022) e1606.

[6] F.N. Fritsch, J. Butland, SIAM J. Sci. and Stat. Comput. 5 (1984) 300–304.

[7] I.T. Jolliffe, J. Cadima, Phil. Trans. R. Soc. A. 374 (2016) 20150202.

[8] W. Windig, S. Markel, Journal of Molecular Structure 292 (1993) 161–170.

[9] E.W. Lemmon, M.O. McLinden, and D.G. Friend, (n.d.).

List of Posters

Morning Poster Session A (10:10 – 11:15)

Number	Name	Title
A1	Meruyert Alisher	*Effect of carbonates on the precipitation of iron hydroxide*
A2	Clelia Bouchaud-Deliot	*Effect of sodium orthophosphate on the rheology and early kinetics of a Mg carbonate cement*
A3	Rachele Butti	*Enhancing the Understanding of Gold Nanoparticle Formation in Ionic Liquids through Variable Temperature In Situ Liquid Phase Scanning Transmission Electron Microscopy*
A4	Arthittaya Chuaybamrung	*Development of Grafted Natural Rubbers Latex Carbon Nanotube Composites and their Mechanical and Electrical Properties*
A5	Ramzi Dakhmouche	*Long-range predictions for Energy Systems*
A6	Lorenzo J. A. Ferraresi	*Thin Film Photodetectors for Time-Resolved Applications*
A7	Marco Finger	*Graphene Nanoribbons as Atomically Precise Light Emitters*
A8	Ali Jafarabadi	*Self-Locking Fe-Based Shape Memory Joints*
A9	Danyang Jiang	*Reconciling plastic release: Comprehensive modeling of macro- and microplastic flows to the environment*
A10	Soumaya Khiari	*Effect of carbonates on the solubility of lepidocrocite*
A11	Raphael Kuhn	*Sodium hexametaphosphate as superplasticizer for MgO-silicate cement stabilized clays*
A12	Xuanchen Li	*Graphene nanoribbons as a quantum platform*
A13	Matteo De Marzi	*Enhancing the external quantum efficiency response under rear illumination in Bifacial CIGS Solar Cells*
A14	Chiara Menegus	*Effect of Hydrogen on the passivity of steels by a surface analytical approach*

A15	Camilla Minzoni	*Reaction Pathway of Copper ALD via Time-of-Flight Mass Spectrometry*
A16	Veronica Montanaro	*Fokker-Planck model for non-equilibrium fluid dynamics*
A17	Manon Murdeu	*Human-based placenta-embryo chip for developmental toxicity assessment of nanoparticles and drugs*
A18	Jorge Sanchez	*Phase behaviour of Cellulose nanocrystals doped with melanin and polydopamine*
A19	Suyash Singh	*Tuning the Exchange Interactions in Triangulene-based Spin Platforms*
A20	Jacopo Sorani	*Redefining Drug Innovation: How to Integrate the Safe and Sustainable by Design (SSbD) Framework to the Pharmaceuticals and Nanomedicines Sector*
A21	Noé Stauffer	*Dynamic optimal model reduction*
A22	Akshat Sudheshwar	*Approaches to Facilitate Environmentally Safe and Sustainable Decision-Making*
A23	Francesco Taddei	*Influence of partial curing on residual stress and process time in Additive Manufacturing of thick thermosetting composites*
A24	Umut Taylan	*Fabrication of Sub-10 µm Size Asymmetric Microstructures by Mask Projection Laser Ablation with Gray Level Transmission Intensities*
A25	Alex Weitnauer	*Airborne mid-infrared spectroscopy for in-situ water vapor isotope measurements in the upper atmosphere*
A26	Valeria Zanrè	*Influence of osteoporosis and COVID-19 on bone microscale properties: A Raman spectroscopy and nanoindentation study*
A27	Cansu Zeytun Karaman	*Ethylsulfone-containing polysiloxanes for dielectric elastomer actuators*
A28	Wolfgang Jan Zucha	*Effect of magnesium-based cementitious binder on smectite for earth construction*

Afternoon Poster Session B (15:30 – 16:30)

Number	Name	Title
B1	Raluca-Ana-Maria Barna	*The Ligamentum Flavum's Role in Spine Degeneration and Aging*
B2	Martina Birocco	*Investigating humidity-driven variations in fracture toughness of alumina via microcantilever testing and Gaussian regression*
B3	Sofiia Butenko	*3D-printed composites with aligned 1D lead-free piezoelectric ceramic fillers for soft self-powered tactile sensors for soft grippers*
B4	Vahid Charkhesht	*The Effect of Graphene on Fast Charging and Discharging Performance of LFP in Li-Ion-Based Supercapacitors*
B5	Shungui Deng	*Insights into the Overcharge-Induced Failure Mechanism of Lithium-Sulfur Batteries*
B6	João Pedro Ferreira Assunção	*Squaraine dye based organic photomultiplication diodes with 220% external quantum efficiency at 1240 nm*
B7	Corentin Foucher	*Multiscale investigation of impact mitigation strategies: Biomimicking musk ox head*
B8	Stefanie Frick	*Accelerating the development of oxynitride coatings using combinatorial magnetron sputtering*
B9	Sebastian Habermann	*Cathodoluminescent and Characteristic X-ray-emissive Rare-Earth-doped Core/Shell Protein Labels for Spectromicroscopic Analysis of Cell Surface Receptors*
B10	Mohammad Jafarpour	*Impact of Cavity Parameters on Gravure Printing for Printed Electronics*
B11	Tino Adrian Jucker	*Clinical evaluation of an innovative air mattress for neonatal pressure ulcer prevention*
B12	Matthias Klimpel	*Unveiling Surface Chemistry of Ultrafast-Sintered LLZO Solid-State Electrolytes for High-Performance Li-Garnet Solid-State Batteries*
B13	Léo Lapeyre	*Exploring Early-Stage Growth Dynamics of LiNbO3 by ALD on NMC 811 Cathodes: an In Situ QCM Analysis for Artificial SEI Applications*

B14	Jincheng Luo	*Scalable Coating of Wide-Bandgap Perovskites on Flexible Substrates for Photovoltaic Application*
B15	Philipp Meier	*Safety and sustainability assessment of antiviral, antibacterial and antifungal nanocoatings applied on porous- and non-porous surfaces*
B16	Ceren Mitmit	*Semi-transparent Wide-Bandgap ACIGS Solar Cells by Low Temperature Processes*
B17	Vittorio Montanelli	*Microstructural Studies of Thin Film All-Solid-State Batteries by S/TEM*
B18	Saketh Ravuri	*Nanographene based building blocks for tailoring magnetic phases*
B19	Sina Ruhstaller	*Prenatal origin of allergies: Can early-life environmental co-exposures to micro-/nanoplastics and allergens induce immune changes at the maternalplacental-fetal interface?*
B20	Hauke Schlesier	*Recycling fossil infrastructure for greener energy transitions*
B21	Katharina Sribike	*A dynamic dECM-based hydrogel for in vitro tissue models*
B22	Dan Stefanita	*Improving local antibiotic therapy through the study of interactions and release mechanisms between CaSO4 carriers and antibiotics*
B23	Xue Sun	*Translating Planetary Boundaries into Material-Level Life Cycle Assessments*
B24	Nikolaos Tagaras	*A nanomedicine challenge under the radar: a case study of Mn@PCN224 nanozyme biotransformation*
B25	Elisabeth Tobler	*Optimizing fresh fruit Supply Chains with Digital Twins*
B26	Ziting Wang	*Silicon carbide nanowires affect respiratory epithelial cell-mediated innate immune defense by impairing mucociliary functions*
B27	Erfu Wu	*A CMOS-Compatible Fabrication Approach for High-performance Perovskite Photodetector Arrays*
B28	Yiwen Zhang	*Using a Dynamic Probabilistic Material Flow Analysis Approach to Capture Japanese Plastic Flows*
B29	Zeyu Zhou	*Effect of aluminium on the hydration and strength of MgO-nesquehonite Binders*

A1. Meruyert Alisher

Effect of carbonates on the precipitation of iron hydroxide

Meruyert Alisher[1], Fabio E. Furcas[1], Barbara Lothenbach[1]*

[1] *Concrete & Asphalt Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

INTRODUCTION: Steel corrosion and the subsequent precipitation of iron hydroxides is a primary factor in the degradation of reinforced concrete structures. Despite extensive focus on iron hydroxides' transformation at low pH, little is known about these processes at high pH and in the presence of cementitious materials. This study focuses on carbonates' effect on iron hydroxides' transformation kinetics. Understanding the effect of carbonates will be an important puzzle piece, unravelling the precipitation of corrosion products in complex aqueous electrolytes.

METHODS: Stock solutions were prepared by mixing 5 mL 1 M $FeCl_3 \cdot 6H_2O$ (in 2% HNO_3) with 245 mL 1 M NaOH to maintain pH=14 and $[Fe_{aq}]$=20 mM. Carbonates were introduced into the solution by adding Na_2CO_3 into 1 M NaOH reaching final concentrations of 0, 10, and 100 mM. Thermogravimetric analysis (TGA) and X-ray diffraction (XRD) were applied to identify the solid iron hydroxides that had formed.

RESULTS & DISCUSSION: XRD and TGA showed the instant formation of 2-line ferrihydrite, $Fe(OH)_3$(s), which slowly transformed into the crystalline corrosion product goethite, FeOOH(s). Minor changes in rate constants (k) were observed at different carbonate concentrations (Fig. 1). Similar studies by Li et al. at pH=10 showed a correlation between carbonate concentration and corrosion product formation, which suggests a need in further studies at moderately alkaline pH [1].

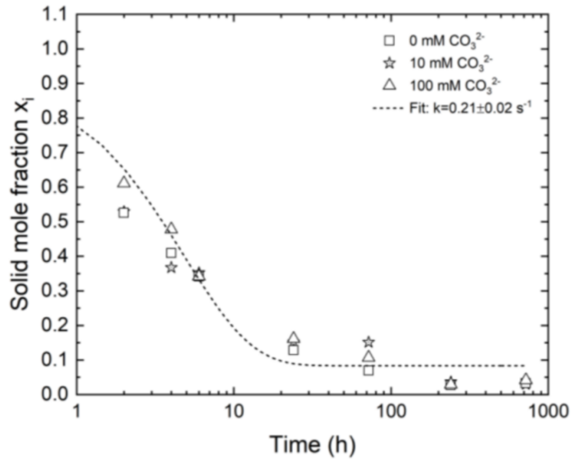


Fig. 1: *Change of 2-line ferrihydrite molar fraction as a function of time and estimated first order rate constants.*

CONCLUSIONS: Carbonates in the concrete pore solution at pH=14 have a negligible effect on corrosion products' transformation. Further studies at intermediary alkaline pH might be necessary to understand the relationship between carbonates and iron corrosion products.

ACKNOWLEDGEMENTS: This work is supported by the Swiss National Science Foundation project no. 10000099: PRINCE.

REFERENCES:

[1] Y. Li, C. Zhang, M. Yang, J. Liu, H. He, Y. Ma, Y. Arai, Effects of carbonate on ferrihydrite transformation in alkaline media, Environ. Sci.Process. & Impacts 26 (2) (2024) 288–297. https://doi.org/10.1039/d3em00469d.

A2. Clelia Bouchaud-Deliot

Effect of sodium orthophosphate on the rheology and early kinetics of a Mg carbonate cement

Clelia Bouchaud-Deliot[1], Frank Winnefeld[1], Barbara Lothenbach[1]

[1] Laboratory for Concrete and Asphalt, Empa, Swiss Federal Laboratories for Materials Sc

INTRODUCTION: Production of cement is responsible for 8% of anthropogenic CO_2 emissions, mainly because of the decomposition of limestone into CaO and CO_2 during the process [1]. Therefore, a solution to reduce CO_2 emissions has to be found. Among the possible options, Mg carbonate cements are a promising alternative. MgO can be extracted from brines or Mg-silicate rocks without releasing chemically bound CO_2. Moreover, it is possible to capture CO_2 through the carbonation of MgO [2]. Therefore, Mg carbonate cements could act as a carbon sink and be a game changer for the cement industry.

However, Mg carbonate cements have a high water demand and short setting times, which negatively affects their workability. Therefore, this study focuses on the role of an additive, sodium orthophosphate, regarding the rheology and the early reaction kinetics of a Mg carbonate cement.

METHODS: The effect of sodium orthophosphate on the rheology of Mg carbonate cement is studied through viscosity and Zeta potential measurements. The reaction kinetics is followed by isothermal calorimetry, and the phases forming at different times are characterized.

RESULTS & DISCUSSION: Viscosity measurements show that sodium orthophosphate improves the rheology of Mg carbonate cement. This is likely due to the increased negative charges related to orthophosphate adsorbing on the particle surfaces, as shown by Zeta potential measurements. Isothermal calorimetry indicates that sodium orthophosphate delay the reaction. This observation is confirmed by phase analysis.

CONCLUSIONS: Sodium orthophosphate is a promising additive to improve the workability and the workability time of Mg carbonate cements.

ACKNOWLEDGEMENTS: This work is supported by the Swiss National Science Foundation through the SNSF Advanced Grants project no. TMAG-2_209222/1.

REFERENCES:

[1] IEA (2018). Technology Roadmap Low-Carbon Transition in the Cement Industry. France/WBCSD, Geneva, Switzerland. IEA, Paris.

[2] Winnefeld, F., Leemann, A., German, A., & Lothenbach, B. (2022). CO_2 storage in cement and concrete by mineral carbonation. Current Opinion in Green and Sustainable Chemistry, 38, 100672.

A3. Rachele Butti

Enhancing the Understanding of Gold Nanoparticle Formation in Ionic Liquids through Variable Temperature In Situ Liquid Phase Scanning Transmission Electron Microscopy

Rachele Butti[1], Debora Keller[1]

[1] Electron Microscopy Center, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

INTRODUCTION: Gold nanoparticles (Au-NPs) are prized for their unique properties, driving advances in catalysis, sensing, and nanomedicine.[1] Ionic liquids (ILs), with their low volatility, high thermal stability, and tunable properties, emerge as ideal media for Au-NP synthesis.[2,3] However, the precise growth mechanisms remain underexplored, limiting application-specific optimization.[4]

METHODS: This study employs variable temperature *in situ* liquid phase scanning transmission electron microscopy (VT LP-STEM) to unravel the dynamics of Au-NP formation in ILs at atomic resolution. Investigations focus on temperature, IL composition, and electron beam effects, using ILs such as 1-butyl-3-methylimidazolium chloride (BMI) and tetrabutylammonium chloride (TBAC). Gold precursors mixed with reducing agents were imaged on MEMS-based heating E-chips, complemented by *ex situ* analyses.

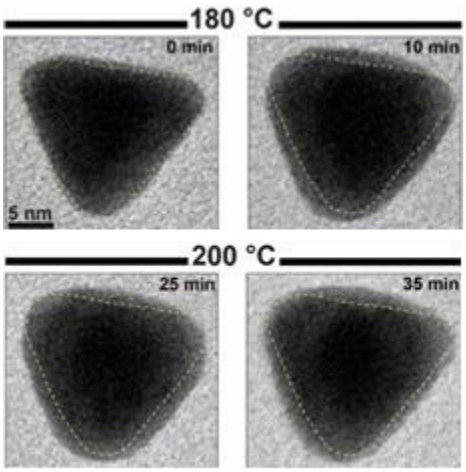


Fig. 1: *In situ STEM series depicting the growth of a triangular-shaped Au-NP in BMI triggered by heat.*

RESULTS & DISCUSSION: Results reveal that IL environment and experimental parameters critically influence NP growth. In BMI, triangular-shaped NPs transitioned to rounded morphologies under elevated temperatures and electron beam irradiation. Conversely, TBAC exhibited negligible growth under similar conditions (Figure 1). *Ex situ* analyses confirmed the size and structure of synthesized NPs, corroborating *in situ* findings.

CONCLUSIONS: This research highlights ILs' potential as versatile media for controlled NP synthesis. VT LP-STEM enables unprecedented insights into nanomaterial growth, advancing eco-friendly and customizable production techniques.[4,5]

Future benefits include the development of sustainable nanomaterial synthesis methods with reduced environmental impact, fostering innovation in green technologies. Overcoming challenges such as electron beam-induced artifacts and scalability issues will pave the way for widespread industrial and societal applications.

ACKNOWLEDGEMENTS: The authors acknowledge financial support from the Swiss National Science Foundation (SNF), Project No. 200021_212177.

REFERENCES:

[1] D. Keller, T.R. Henninen, R. Erni, Nanoscale 12 (2020) 22511–22517.

[2] V. Khare, C. Ruby, S. Sonkaria, A. Taubert, Int. J. Precis. Eng. Manuf. 13 (2012) 1207–1213.

[3] H. Duan, D. Wang, Y. Li, Chem. Soc. Rev. 44 (2015) 5778–5792.

[4] H. Zheng, R.K. Smith, Y. Jun, C. Kisielowski, U. Dahmen, A.P. Alivisatos, Science 324 (2009) 1309–1312.

[5] D. Alloyeau, W. Dachraoui, Y. Javed, H. Belkahla, G. Wang, H. Lecoq, S. Ammar, O. Ersen, A. Wisnet, F. Gazeau, C. Ricolleau, Nano Lett. 15 (2015) 2574–2581.

A4. Arthittaya Chuaybamrung

Development of Grafted Natural Rubbers Latex Carbon Nanotube Composites and their Mechanical and Electrical Properties

Arthittaya Chuaybamrung[1], Rawiporn Promsung[1], Ekwipoo Kalkornsurapranee[1], Yeampon Nakaramontri[2]*, Frank Clemans[3]*

[1] *Division of Physical Sciences, Faculty of Science, Prince of Songkla University, Songkhla, Thailand*

[2] *Sustainable Polymer & Innovative Composites Material Research Group, Faculty of Science, King Mongkut's University of Technology Thonburi, Bangkok, Thailand*

[3] *Laboratory for High Performance Ceramics, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

INTRODUCTION: Conductive elastomers are elastic materials designed to transmit electricity, often made from natural rubber (NR) or similar alternatives by incorporating conductive materials. NR is a renewable material known for its outstanding elasticity, resilience, and tensile strength [1]. NRcomposites reinforced with carbon nanotubes (CNT) enhance mechanical and electrical properties, though uniform CNT dispersion is challenging due to strong Van der Waals forces and their high aspect ratio [2]. Improving the nteraction between CNT and NR is key to enhancing composite performance. Several studies have focused on these enhancements, and it is known that modification of NR is a choice to overcome its drawbacks [3,4]. Therefore, this study focuses on enhancing the mechanical and electrical properties of NR-CNT composites by grafting functional groups onto NR molecules. This study introduces a novel method for producing conductive grafted NR-CNT latex films using an easy casting process with glutaraldehyde crosslinking agent, enhancing electrical sensing properties.

METHODS: The grafted NR was performed via redox emulsion polymerization. Grafting efficiency was confirmed through Soxhlet extraction, and copolymerization was verified by 1H–NMR and ATR–FTIR. CNTs were added as conductive fillers, mixed by sonication, and cured with glutaraldehyde curing agent. Finally, properties in terms of modulus, tensile strength, electrical conductivity and piezoresistive sensor behaviour were investigated.

RESULTS & DISCUSSION: The tensile properties of CNT filled grafted NR composites were investigated in terms of modulus, tensile strength and elongation at break. There is a significant change in the deformation behaviour of cured grafted NR upon the addition of CNT. Furthermore, the filler–filler interaction of the grafted NR/CNT composites was elucidated by the dynamic tensile testing between 0–100 % strain during 10 cycles. It is observed that the maximum stress of the grafted NR/CNT composites significantly decreased after the 1^{st} cycle of dynamic tensile test. This is due to the dissociation of filler–filler interaction of CNT led to the decreasing of maximum stress in each cycle [3]. This is attributed to the higher energy dissipation caused by the filler–filler interaction in the composites. The mechanical hysteresis behaviour is well related to increasing the CNT filler content. The electrical conductivity increased and later (CNT > 2 phr) decreased by increasing the CNT content. The higher filler–filler interaction resulted in lower mechanical properties due to the self–agglomeration of CNT above 2 phr [4].

CONCLUSIONS: The composites of grafted NR cured with glutaraldehyde and various CNT contents were prepared by casting process. The grafted NR-CNT composites, cured with glutaraldehyde offer an energy-efficient, environmentally friendly method for the development of flexible soft robotic sensor.

ACKNOWLEDGEMENTS: This research project is also supported by National Research Council of Thailand (NRCT): (N41A640236).

REFERENCES:

[1] Alarifi, J. Mater. Res. Technol. 8 (2019) 4863-4893.

[2] Zhao, et al. A review, Eng. Struct. 210 (2020) 110339.

[3] Nakaramontri, et al. Rubber Chem. Tech. 89 (2016) 272-291.

[4] Promsung, et al. Discover Nano 19 (2024) 30.

A5. Ramzi Dakhmouche

Long-range predictions for Energy Systems

Ramzi Dakhmouche[1], Ivan Lunati[1], Hossein Gorji[1*]

[1] *Laboratory for computational Engineering, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

INTRODUCTION: Energy markets are structured according to purchasing time-scale, i.e. prices vary significantly depending on whether the energy is to be consumed sooner or later. Hence, energy providers need demand forecasting models which are accurate in capturing long-range dependencies, which is also known as extrapolation. Furthermore, such models should be robust to distribution shift to be applicable to various regions.

METHODS: Current state-of-the-art machine learning models do not capture long-range dependencies [1, 2], i.e. they are not able to extrapolate. We propose a novel scalable method to address that which builds upon symbolic regression. Symbolic regression consists in leveraging data to find an accurate model among a rich set of non-linear functions [3].

RESULTS & DISCUSSION: Our numerical experiments show that the method has promising performance. In particular, it performs very well in the low data regime, which demonstrates its practical utility, as data is often costly to acquire and clean, in industrial settings.

CONCLUSIONS: The method we proposed is scalable data-driven approach to perform long-range forecasts for energy systems with renewable energy sources. It tackles a practical challenge, faced by energy providers in an uncertain environment with renewable energy sources.

ACKNOWLEDGEMENTS: The first author acknowledges funding under Swiss National Science Foundation under grant No. 212876.

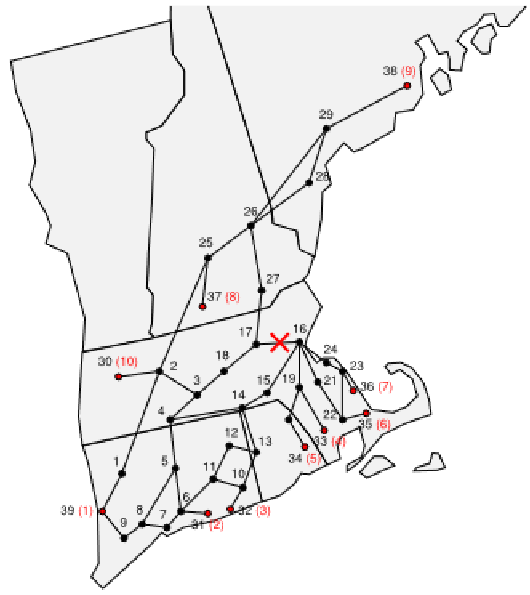


Fig.1: New England Electrical Grid Network

REFERENCES:

[1] Zhaozhi Qian, Krzysztof Kacprzyk, and Mihaela van der Schaar. D-code: Discovering closed-form odes from observed trajectories. In International Conference on Learning Representations, 2022.

[2] Ramzi Dakhmouche, Ivan Lunati, and Hossein Gorji. Robust symbolic regression for network trajectory inference. In ICLR 2024 Workshop on MLGenX.

[3] Steven L Brunton, Joshua L Proctor, and J Nathan Kutz. Discovering governing equations from data by sparse identification of nonlinear dynamical systems. Proceedings of the national academy of sciences, 2016.

A6. Lorenzo J. A. Ferraresi

Thin Film Photodetectors for Time-Resolved Applications

Lorenzo J. A. Ferraresi[1,2], Ivan Shorubalko[1*]

[1] Transport at Nanoscale Interfaces, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

[2] Department of Chemistry and Applied Biosciences, ETH – Swiss Federal Institute of Technology Zürich, Zürich, Switzerland

The advancement of autonomous machinery relies on tools capable of perceiving their surroundings through light-based technologies such as image recognition, visible light communication, and light ranging. These applications demand photodetectors with high efficiency, rapid response times, seamless integration, and low fabrication costs—requirements well addressed by thin-film photodetectors.

Our work investigates two classes of solution-processed materials: hybrid lead halide perovskites (LHPs, specifically $(Cs_{0.14}FA_{0.86})Pb(Br_{0.14}I_{0.86})_3$) and colloidal quantum dots (cQDs, specifically PbS and InAs). While significant progress has been made in enhancing detectivity in the visible (LHPs) and infrared (cQDs) ranges, response time remains underexplored despite its critical role in enabling time-resolved applications.

Two strategies are pursued: device engineering to minimize the resistance-capacitance (RC) time constant and material chemistry to fine-tune intrinsic material properties. Cleanroom fabrication techniques are employed to achieve optimized device architectures, targeting picosecond-scale response times for InAs cQD devices. Additionally, electro-hydrodynamic (EHD) printing enables precise deposition of PbS cQDs, followed by ligand exchange in printed pixels[1]. For LHPs, stoichiometric control enhances response speeds by an order of magnitude. For cQDs, surface ligand selection during synthesis plays a decisive role.

Material characterization employs spectroscopy techniques (XRD, EDX, PL, absorbance) and specialized tools such as AFM-IR for printed cQD pixels. Advanced device characterization, including time- and temperature-resolved photocurrent measurements, provides insights into carrier dynamics.

These studies highlight the synergy between device engineering and material chemistry, driving thin-film photodetectors towards time-resolved applications and advancing their integration into future autonomous systems.

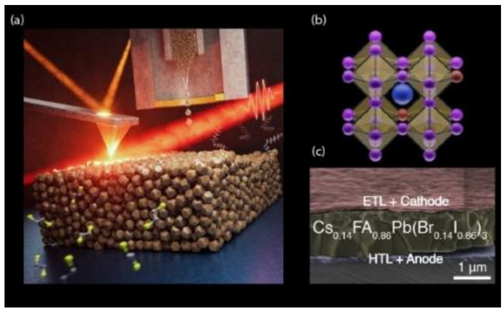


Fig. 1: *Colloidal quantum dots and perovskites for fast and sensitive thin film photodetectors. (a) Depiction of EHD printing of PbS cQDs pixels and AFM-IR analysis of their ligand exchange process (b) Depiction of the crystal structure of the typical perovskite compound used for devices (c) SEM cross-section of a thin film photodiode with perovskite absorber layer.*

REFERENCES:

[1] L. J. A. Ferraresi, G. Kara, N. A. Burnham, R. Furrer, D. N. Dirin, F. La Mattina, M. V. Kovalenko, M. Calame, I. Shorubalko, *Nano Lett.* **2024**, *24*, 10908.

A7. Marco Finger

Graphene Nanoribbons as Atomically Precise Light Emitters

M. Finger[1,2], D. Dutta[1], A. Ortega[1], M. Perrin[2,3], R. Fasel[1,4], G. Borin Barin[1]

[1] *nanotech@surfaces Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Department of Information Technology and Electrical Engineering, ETH Zürich, Zürich, Switzerland*

[3] *Transport at Nanoscale Interfaces Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[4] *Department of Chemistry, Biochemistry and Pharmaceutical Sciences, University of Bern, Bern, Switzerland.*

INTRODUCTION: On-surface synthesis allows to fabricate graphene nanoribbons (GNRs) with atomically precise structures. This degree of synthetic control is achieved through selective surface-catalyzed reactions in well-designed molecular precursors[1,2]. The rich chemical space afforded by the precursors allows to strategically incorporate structural motifs into GNRs to engineer their opto-electronic properties[3]. GNRs can be designed to be stable yet atomically precise light emitters whereas the emission wavelength can be tuned by changing their chemical structure[4]. This makes atomically precise GNRs promising active materials in opto-electronic devices.

MOTIVATION: Recently, Jiang et al. observed sharp excitonic light emission from a single, electronically decoupled seven-atom-wide armchair edge GNR (7-aGNR) by STM-Luminescence (STML)spectroscopy. The light emission was more efficient over the termini of the 7-aGNR which host localized electronic state[5]. However, these states are quenched when the ribbon termini are contacted in a device, making them inaccessible for device integration.

PERSPECTIVE: We present a potential solution to this obstacle through localized electronic states on structural motifs (edge extensions, electron donor-acceptor groups, heteroatoms) to provide a robust platform for luminescence. We revisit the on-surface synthesis of a well-known derivative of the 7-aGNR, featuring periodic zigzag edge extensions[6,7], to mimic the luminescent end states within the bulk GNR. To incorporate luminescent GNRs into opto-electronic devices, a transfer step from the growth-surface onto a non-metallic substrate is necessary to prevent luminescence quenching. We investigate how the Raman spectra differ between various known GNR modifications and their evolution with environmental parameters (gas partial pressure, temperature) to characterize their structural integrity across different transfer steps.

ACKNOWLEDGEMENTS: Funding from SNF project no 219172 (Graal) is greatly acknowledged.

REFERENCES:

(1) J. Cai et al., Nature 466, 470–473 (2010)

(2) L. Talirz et al., Adv. Mater. 28, 6222–6231 (2016)

(3) R. S. K. Houtsma et al., Chem. Soc. Rev. 50, 6541–6568 (2021)

(4) X. Wu et al., Phys. Chem. Chem. Phys. 22, 8277−8283 (2020)

(5) S. Jiang et al., Science 379, 1049–1054 (2023)

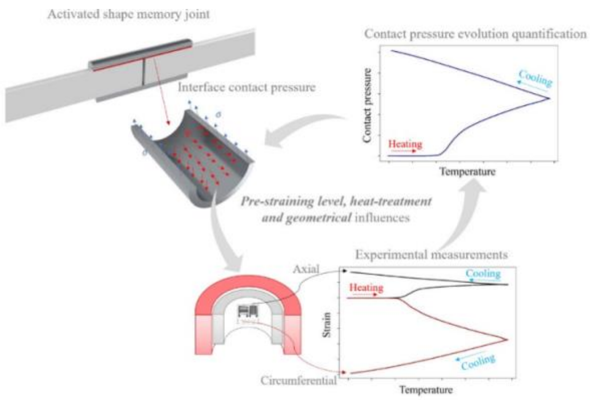
(6) Q. Sun et al., Nano Lett. 20, 6429−6436 (2020)

(7) D. J. Rizzo et al., Science 369, 1597–1603 2020)

A8. Ali Jafarabadi

Self-Locking Fe-Based Shape Memory Joints

Fe-based Shape memory alloys (Fe-SMAs) have been extensively utilized in a variety of innovative engineering applications. Notably, Fe-based shape memory couplers present an alternative to welded and machined mechanical joints, offering advantages such as self-locking assembly and reduction of stress concentrations. However, further characterization in terms of multiaxial shape memory effect (SME) and, geometrical as well as implementation parameters is crucial for the purpose of reliable strength evaluation. While significant progress has been made toward understanding the uniaxial characteristics of the SME—driven by major developments and widespread use of such materials—the behaviour of Fe-SMAs under complex loading conditions, such as those involving multiaxial phase transformations, remains less well understood. During the pre-straining process of Fe-SMA tubes, nonuniform biaxial stress-state leads to a complex stress-induced martensite formation, posing challenges in the assessment of SME. Nonetheless, it is feasible to interpret the overall SME performance based on the resultant pressure exerted by the Fe-SMA tube on a substance, thereby limiting its free recovery. This study explores the impact of heat-treatment, pre-straining level, activation temperature and wall-thickness on interface contact pressure, providing insights into the gripping capacity in Fe-SMA tubes, which is crucial for evaluating the strength of shape memory joints. Via coupling of analytical models with results extracted from an experimental campaign, the resultant pressure at the interface throughout the course of activation is quantified, aiding to assess the SME performance. The obtained results highlight the complex interaction between post-processing and structural parameters, shedding light on the design and implementation of Fe-SMA coupling components with enhanced SME performance.



A9. Danyang Jiang

Reconciling plastic release: Comprehensive modeling of macro- and microplastic flows to the environment

Danyang Jiang[1], Bernd Nowack[1]

[1] *Technology and Society Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, Switzerland*

INTRODUCTION: Plastic emissions is one of the major environmental issues of the 21st century. Material flow analysis combined with release assessments is one way to quantify plastic emissions from a whole product life cycle perspective. However, current plastic release models contain significant gaps and need improvement, particularly in important emission pathways such as littering, construction wastes and textile washing.

METHODS: This study integrated recent research on key emission pathways into a plastic release model based on probabilistic material flow analysis. We comprehensively modeled macro- and microplastic emissions of seven polymers in Switzerland for 2022.

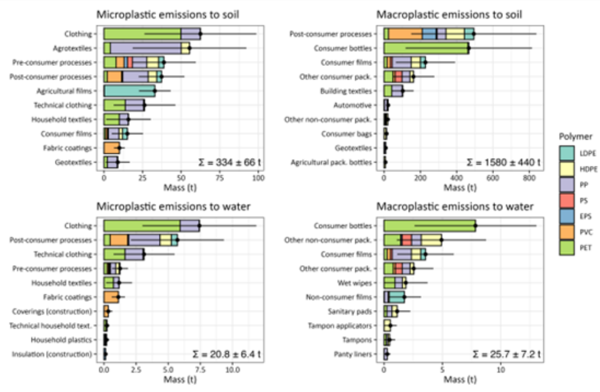


Fig. 1: Macro- and microplastic emissions to soil and water by product in tonnes per year and their polymer composition in Switzerland for 2022. The top ten product categories are shown in this figure.

RESULTS & DISCUSSION: Our model estimates that 222 ± 50 g/capita/year plastics are released into the environment. Fiber release from textiles and pellet loss during pre- and post-consumer processes were identified to be primary microplastic release pathways. For macroplastics, the main release processes are littering of packaging products and losses during post-consumer collection. Soil is identified as the primary receiving compartment for plastic emissions, accounting for 98% of macroplastics and 94% of microplastics, respectively.

CONCLUSIONS: Release models are crucial for predicting concentrations and identifying hotspots of emissions into the environment. Our model offers comprehensive release data across human society. Based on the research gap in large-scale polymer concentration prediction, we emphasize the importance of combining release models with transport and fate models.

A10. Soumaya Khiari

Effect of carbonates on the solubility of lepidocrocite

Soumaya Khiari[1], Fabio Enrico Furcas[1], George-Dan Miron[2], Barbara Lothenbach[1]

[1] *Laboratory for Concrete and Asphalt, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Laboratory for Waste Management, Paul Scherrer Institute PSI, Center for Nuclear Engineering and Sciences, Villigen, Switzerland*

INTRODUCTION: Steel reinforcement corrosion is a major factor limiting the service life and durability of reinforced concrete structures. The processes occurring at the steel-concrete interface are critical. Despite their significance in corrosion mechanisms, the behavior of iron species in high-pH cementitious environments remains poorly understood. A recent study [1] has indicated that carbonates could increase the solubility of iron hydroxides at high pH values, which is investigated in this research.

METHODS: Lepidocrocite (γ-FeOOH) was synthesized under controlled conditions and characterized using X-ray diffraction (XRD) and thermogravimetric analysis (TGA). Solubility studies were conducted at 20°C from undersaturation experiments in highly alkaline solutions (pH 14) with varying carbonate concentrations: 0, 1, 10, 20, 50, and 100 mM equilibrating between 1 and 38 days. Fe concentrations were determined by inductively coupled plasma optical emission spectroscopy (ICP-OES).

RESULTS & DISCUSSION: The iron concentration in equilibrium with lepidocrocite increases strongly with pH due to the formation of aqueous $Fe(OH)_4^-$. The measured concentrations were slightly lower than the predicted lepidocrocite solubility (Fig. 1). The variability of the measurements will be further investigated. The presence of carbonate has no significant effect on its solubility, indicating that no or only weak $Fe(OH)_4^-$-carbonate complexes are present in the solution at pH 14. The potential formation of $Fe(OH)_4^-$-carbonate complexes will be further investigated at lower pH values.

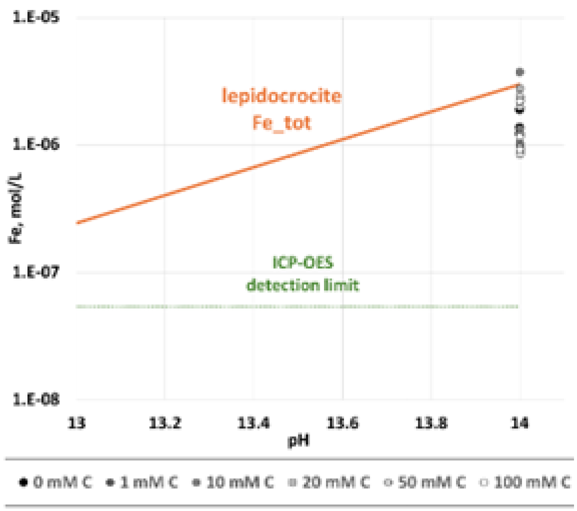


Fig. 1: *Effect of carbonate on the solubility of lepidocrocite. The calculated solubility of lepidocrocite is indicated by the solid line, measurements by circles; the color indicates the carbonate concentration: Black: 0 mM, white: 100 mM)*

CONCLUSIONS: The experimental solubility data indicate that the solubility of lepidocrocite at pH 14 is not significantly influenced by the presence of carbonates.

ACKNOWLEDGEMENTS: This work is supported by the Swiss National Science Foundation project no. 10000099: PRINCE.

REFERENCES:

[1] E. Wieland, G. D. Miron, B. Ma, et al., Speciation of iron(II/III) at the iron-cement interface: A review, Mater. Struct. 2023, 56, 31.

A11. Raphael Kuhn

Sodium hexametaphosphate as superplasticizer for MgO-silicate cement stabilized clays

Raphael Kuhn[1,2], Pietro Lura [1,2], Guillaume Habert [3], Ellina Bernard [1]

[1] Concrete and Asphalt, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

[2] Swiss Federal Institute of Technology (ETH Zürich), Institute for Building Materials (IfB), Zürich, Switzerland

[3] Swiss Federal Institute of Technology (ETH Zurich), Institute of Construction and Infrastructure Management (IBI), Zürich, Switzerland

ABSTRACT: Achieving a good workability of clay-based building materials during mixing and placing is a key factor when building strong and durable structures. However, the fluidity of clay mineral based materials is impaired by stabilization with hydraulic binders such as Portland-based cement. While stabilization is essential to increase the mechanical properties and therefore cannot be omitted, it is possible to reduce the viscosity of the material with superplasticizers. Common clay superplasticizers as sodium hexametaphosphate (NaHMP) are incompatible with Portland based cement, namely they considerably retard Portland cement hydration. Hence, stabilizers that are both compatible with clays and superplasticizers must be sought.

In this study, the combination of NaHMP and MgO-silicate cement is tested as a potential superplasticizer and stabilizer for clay-rich materials. The influence on the rheology is investigated by slump tests and rheometer measurements. The mechanism of action is analyzed based on the particle interactions using zeta potential and static light scattering (SLS). The sorption behavior of the superplasticizer is determined by ^{31}P MAS NMR and pore solution analysis (ICP-OES, TOC, and pH). It is shown that NaHMP adsorbs as a polyphosphate with different chain lengths. The polyphosphates induce an increased negative surface charge on the particles, which leads to a strong electrostatic repulsion. This repulsion in turn reduces the forces that have to be overcome to fluidify the material and allows to achieve the desired workability during casting of structural elements.

A12. Xuanchen Li

Graphene nanoribbons as a quantum platform

Xuanchen Li [1,3], Amogh Kinikar [1], Jeong Ha Hwang [1,3], Nicolò Bassi [1,4], Mickael Lucien Perrin [2,3], Roman Fasel [1,4], Gabriela Borin Barin [1]

[1] *nanotech@surfaces, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Transport at Nanoscale Interfaces, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[3] *ETH Zürich, Zürich, Switzerland*

[4] *University of Bern, Bern, Switzerland*

INTRODUCTION: The constant need for the miniaturization of transistors has driven advancements in transistor scalability and the corresponding computational power. But this downscaling is approaching physical limits for traditional semiconductors, requiring alternative materials and technologies for further scaling [1].

Graphene nanoribbons (GNRs), which are narrow strips of graphene, offer tunable electronic and magnetic properties through precise structural control, positioning them as promising candidates for miniaturized electronic and spintronic applications. Despite their potential, research into GNR-based devices is still in its early stages [2].

METHODS: This talk provides an overview of the on-surface synthesis (OSS) method enabling the fabrication of GNRs with tailored structures, allowing us to uncover diverse quantum behaviors such as topological states and localized spins [3,4].

Various techniques including scanning tunneling microscopy, scanning tunneling spectroscopy, Raman spectroscopy, and others are used to investigate the structural and quantum properties of these on-demand GNRs for potential applications in future quantum technologies.

RESULTS & DISCUSSION: This work discusses our recent progress in optimizing the growth of 17-armchair GNRs and the exploration of a new chiral GNR motif aimed at improving the integration of these GNRs into devices. These advancements demonstrate the potential of GNRs to bridge the gap toward scalable quantum technologies.

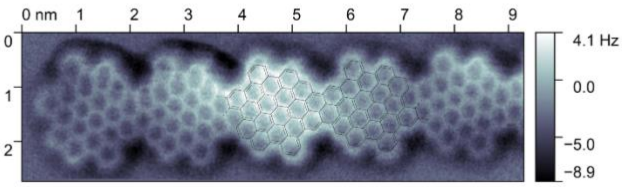


Fig. 1: *Model of the chiral GNR overlaid on the non-contact atomic force microscopy image.*

CONCLUSIONS: By highlighting the critical role of tailored GNR structures, this research provides a foundation for advancing GNR-based quantum devices and underscores their promise for future quantum applications.

REFERENCES:

[1] P. Avouris, Z. Chen, V. Perebeinos, Nature Nanotech 2 (2007) 605–615.

[2] H. Wang, H.S. Wang, C. Ma, L. Chen, C. Jiang, C. Chen, X. Xie, A.-P. Li, X. Wang, Nat Rev Phys 3 (2021) 791–802.

[3] O. Gröning, S. Wang, X. Yao, C.A. Pignedoli, G. Borin Barin, C. Daniels, A. Cupo, V. Meunier, X. Feng, A. Narita, K. Müllen, P. Ruffieux, R. Fasel, Nature 560 (2018) 209–213.

[4] A. Kinikar, X. Xu, M.D. Giovannantonio, O. Gröning, K. Eimre, C.A. Pignedoli, K. Müllen, A. Narita, P. Ruffieux, R. Fasel, Advanced Materials 35 (2023) 2306311.

A13. Matteo De Marzi

Enhancing the external quantum efficiency response under rear illumination in Bifacial CIGS Solar Cells

Matteo De Marzi[1], Nisika[1], Ceren Mitmit[1], Matthias Diethelm[1], Romain Carron[1]

[1] Laboratory for Thin Films and Photovoltaics, *Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

INTRODUCTION: In the past year, thin film (Ag,Cu)(In,Ga)Se_2 solar cells have reached a new record efficiency of 23.6% [1]. Bifacial solar cells have been introduced to boost the yearly yield of solar installations. This enhancement is achieved by harvesting the stray light reflected from the ground (albedo), thereby increasing the photocurrent and power generation.

METHODS: TCOs are implemented as back contact, replacing the opaque molybdenum. Among numerous TCOs, ITO is widely used as a back contact. However, low mobility and high carrier concentration of ITO lead to significant losses. In the present study, we investigate the potential to enhance solar cell performance under rear illumination using a different TCO and band gap engineering.

RESULTS & DISCUSSION: The application of high mobility and low carrier concentration TCO improves the device optics under rear illumination and allows the rear EQE to surpass 80% at infrared wavelength.

Modification of the band gap brings an increase of ~10-15% of the EQE response at low wavelengths, compared to standard cells, improving the short-circuit current (Jsc) from the rear by about 3 mA/cm2.

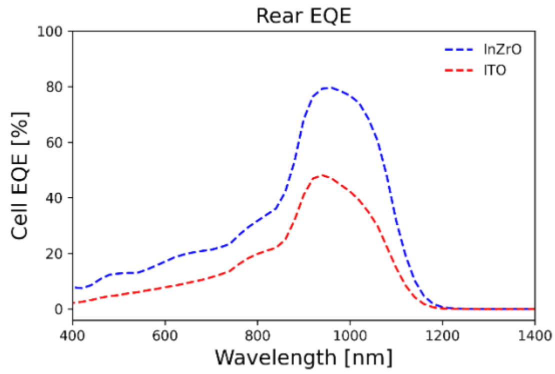


Fig. 1: External quantum efficiency response under rear illumination for two cells with different TCOs: ITO and InZrO.

CONCLUSIONS: This study offers a potential strategy to improve the performance of bifacial solar cells under rear illumination by TCO selection and band gap engineering. This is one step towards developing bifacial solar cells that are able to overcome the limits of standard devices.

ACKNOWLEDGEMENTS: Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or CINEA. Neither the European Union nor the granting authority can be held responsible for them (Project 101122203 "Hi-BITS").

REFERENCES:

[1] J. Keller, K. Kiselman, O. Donzel-Gargand, N.M. Martin, M. Babucci, O. Lundberg, E. Wallin, L. Stolt, M. Edoff, Nat Energy 9 (2024) 467–478.

A14. Chiara Menegus

Effect of Hydrogen on the passivity of steels by a surface analytical approach

C. Menegus, J.P. Kollender, L.P.H. Jeurgens, C. Cancellieri

EMPA, Laboratory for Joining Technologies and Corrosion, Dübendorf, Switzerland

As we embrace a hydrogen-driven society, we must confront a relevant number of challenges arising from hydrogen interaction with steel across various stages of production, storage, and transportation. Furthermore, the generation and adsorption of hydrogen are unavoidable in many processes such as pickling, cathodic protection, and galvanizing.

While hydrogen embrittlement has been extensively studied, the role of the passive oxide layer naturally forming on steel surfaces is still unclear. This layer not only can protect steel from corrosion but also serves as a barrier against hydrogen penetration.

This study presents a methodology using soft and hard X-ray photoelectron spectroscopy (XPS/HAXPES) to investigate hydrogen's impact on passivated steel. Thermal oxidation is employed to passivate samples, prepared in combinatorial ultra-high vacuum (UHV) facilities for thin-film deposition and post-processing. An electrochemical flow cell charges hydrogen on one sample side, maintaining an inert argon atmosphere on the opposite side to prevent surface polarization and unintended modifications.

Post-charging, samples are analyzed in-situ using XPS/HAXPES to determine oxide layer thickness, composition, oxide/hydroxide phases, Fe^{3+}/Fe^{2+} ratios, and the chemical states at the alloy/oxide interface. Soft and hard X-rays enable nondestructive depth profiling and avoid interference from overlapping Auger lines. Energy shifts in Auger and photoelectron peaks are correlated with reference samples of pure metals and oxides for comparison.

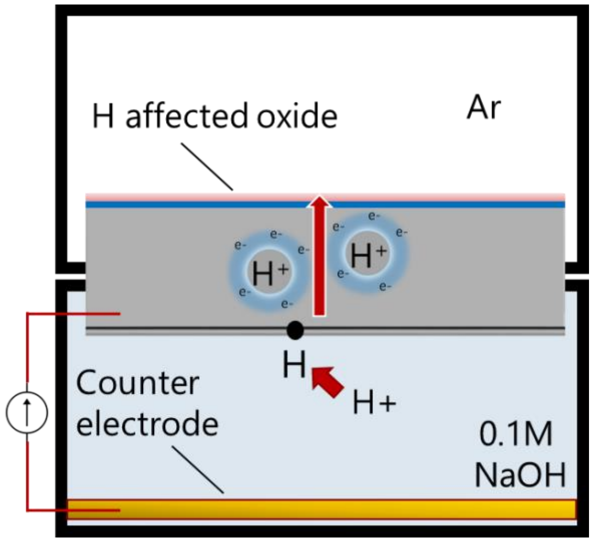


Figure 1. Scheme of the charging cell

This approach provides insights into the complex processes of hydrogen penetration, diffusion, and solubility within the surface layer of steel, contributing to a deeper understanding of hydrogen interactions with passivated steel materials.

A15. Camilla Minzoni

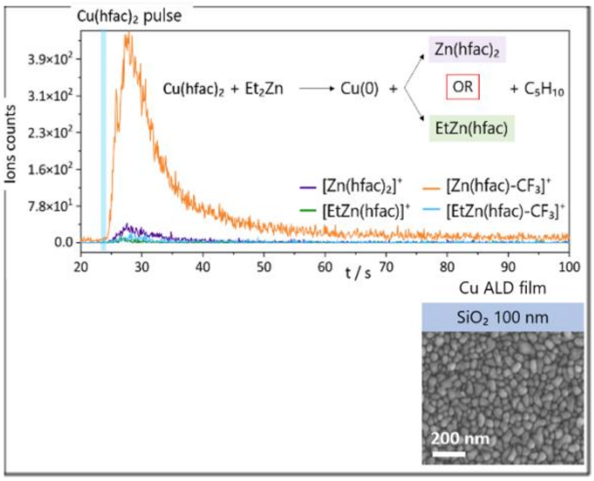
Reaction Pathway of Copper ALD via Time-of-Flight Mass Spectrometry

Camilla Minzoni[1], Caroline Hain[1], Krzysztof Mackosz[1], Abdel Bensaoula[2], Patrick Hoffmann[3], Ivo Utke[1]

[1] *Laboratory for Mechanics of Materials & Nanostructures, Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland*

[2] *Tofwerk, Thun, Switzerland*

[3] *Advanced Materials Processing, Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland*



INTRODUCTION: The current trend towards electronic device miniaturization has made Atomic Layer Deposition (ALD) crucial for next-generation fabrication, particularly for the deposition of uniform and conformal copper thin films. [1].

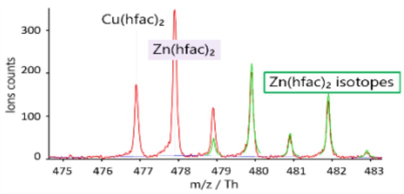


Figure 1. Top: Time-resolved MS spectrum showing reaction by-products. Bottom: $Zn(hfac)_2$ MS. Cu ALD SEM image.

However, applying ALD to metals presents challenges, primarily attributed to the lack of the mechanistic understanding of the surface reactions. [2]

METHODS: This study presents in-situ Time-of-Flight Mass Spectrometry (ToFMS) monitoring to investigate the mechanism involved in the Cu ALD process, using $Cu(hfac)_2$ (hfac=$C_5HF_6O_2$) and diethylzinc DEZ (Et_2Zn) as reducing agent.

RESULTS & DISCUSSION: Two distinct reaction pathways have been proposed for Cu deposition. Lee et al. [3] proposed a complete transmetalation reaction with $Zn(hfac)_2$ formation, while Elliott et al. [4] suggested a half ligand exchange mechanism producing EtZn(hfac). Both mechanisms ultimately yield copper metal and butane (Fig. 1).

During the ToFMS monitoring of the ALD cycles, the theoretically anticipated by-products from both two reactions were detected at different times, leading to a more complex overall reaction path.

CONCLUSIONS: These results are the first of their kind under vacuum ALD conditions, providing experimental evidence for both proposed reaction mechanisms, while supporting also theoretical calculations and solution-based of analogue reactions [4-5].

The combination of ALD and ToFMS is a powerful method for industrial applications, providing a quick and detailed understanding of complex ALD reactions.

ACKNOWLEDGEMENTS: This work is supported by the SNF funding.

REFERENCES:

[1] K. Venkatraman, Electrochem. Comm. 91 (2018).

[2] D. Hagen, Appl. Phys. Rev. 6 (2019) 041309.

[3] B. Lee, Chem. Int. Ed. 48 (2009).

[4] S. Elliott, Chem. Mater. 28 (2016) 17.

[5] B. Vidjayacoumar, Chem. Mater. 22 (2010) 17.

A16. Veronica Montanaro

Fokker-Planck model for non-equilibrium fluid dynamics

Veronica Montanaro[1], Hossein Gorji[1]

[1] Laboratory for Scientific Computing, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

INTRODUCTION: Fluid dynamics in extreme conditions, such as near vacuum, high temperature, and/or hypersonic scenarios remain a difficult topic for conventional Computational Fluid Dynamics. This is because the Navier-Stokes-Fourier equations do not describe the flow accurately anymore [1]. While the kinetic theory provides a proper starting point to deal with such flow phenomena, the numerical tools in our disposal remains largely limited. In recent years, Fokker-Planck based approximations have been developed (mostly heuristically) as diffusive approximations of the Boltzmann kinetic equation, where the collisions are modeled through random noise. Therefore^, significant computational efficiency is gained by approximating discrete collisions underlying the Boltzmann equation via continuous stochastic models [2,3,4].

METHODS: We present a general strategy to construct stochastic models for fluid flows far from the thermal equilibrium. We present a novel Fokker-Planck model which honours prescribed moment dynamics along with the entropy constraint. While the former ensures recovery of correct conservation laws, and thus Navier-Stokes-Fourier system in the continuum limit, the latter leads to the model stability for an arbitrary distribution function.

RESULTS & DISCUSSION: We present results on the model applied to hypersonic shocks, in particular within the setting of a flow of Argon at Mach 5 over a plate. We test the model with various relaxation rates and compare it with results of the state-of-the-art Fokker-Planck models.

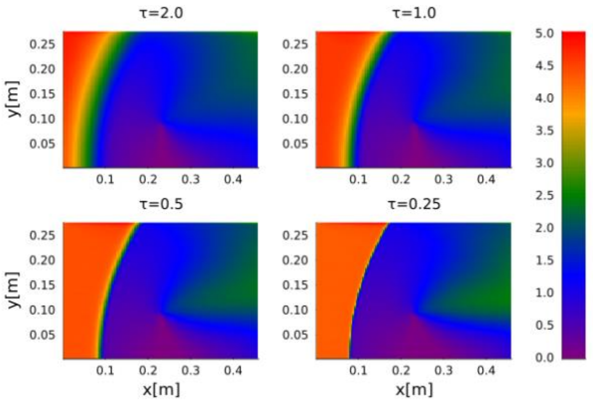


***Fig. 1:** Contour plots of Mach number on the spatial domain, showing different shock thickness for different relaxation rates.*

CONCLUSIONS: By controlling the entropy rate, we develop stochastic particle-based models leading to accurate treatment of non-equilibrium shock scenarios. This important property, along with the efficient handling of particle evolution, uniquely position the proposed model for efficient simulations of non-equilibrium gas processes.

ACKNOWLEDGEMENTS: This work was supported in part by Swiss National Science Foundation under grant 217408.

REFERENCES:

[1] S. Chapman, T.F. Cowling, The Mathematical Gazette 38 (1954) 63–64.

[2] P. Jenny, M. Torrilhon, S. Heinz, Journal of Computational Physics 229 (2010) 1077–1098.

[3] M.H. Gorji, M. Torrilhon, P. Jenny, J. Fluid Mech. 680 (2011) 574–601.

[4] M.H. Gorji, M. Torrilhon, Journal of Computational Physics 430 (2021) 110034.

A17. Manon Murdeu

Human-based placenta-embryo chip for developmental toxicity assessment of nanoparticles and drugs

Manon Murdeu[1], Vera Kissling[1], Jacob Folz[3], Andreas Hierlemann[2], Julia Alicia Boos[2]*, Tina Buerki-Thurnherr[1]*

[1] *Nanomaterials in Health, Empa, Swiss Federal Laboratories for Materials Science and Technology, Lerchenfeldstrasse 5, 9014 St.Gallen, Switzerland.*

[2] *Bioengineering Laboratory, Department of Biosystems Science and Engineering, ETH Zürich, Klingelbergstrasse 48, 4056 Basel, Switzerland.*

[3] *Department of Health Sciences and Technology, ETH Zürich Universitätstrasse 2, 8092 Zürich, Switzerland.*

INTRODUCTION: The lack of data on the potential developmental toxicity of emerging drugs, nanoparticles (NPs) and environmental pollutants has raised safety concerns. This together with the urge of replacing animal testing, highlighted the need of new advanced models to mimic the maternal-embryonic axis. To enable embryotoxicity assessment of different compounds we aim to establish a human-based placenta-embryo chip combining a placental barrier model and an embryoid body (EB) within a single platform.

METHODS: The pump-free microfluidic device features a maternal and embryonic side, separated by a porous membrane in a hanging-drop configuration. To model the placental barrier, a co-culture of primary cytotrophoblast cells (CTBs)-derived from human term placenta and human placental vascular endothelial cells (HPVECs) was developed, while human induced pluripotent stem cells (hiPSCs)-derived EB served as a model for early embryonic development.

RESULTS & DISCUSSION: We achieved the formation of a tight and functional placental barrier featuring a spontaneously syncytialized trophoblast layer as demonstrated by immunohistochemical stainings, EM images, hCG production and size-dependent exclusion of permeability markers. To verify the placenta model, translocation of different NPs and drugs was compared to ex-vivo placenta perfusion studies. Furthermore, EBs maintained viability and capacity for germ-layer differentiation under dynamic exposure on chip. The placenta-EB co-culture was verified with preliminary assessment of known embryotoxic compounds.

CONCLUSIONS: The model will help to gain early pre-clinical data for drug and NP effects, contributing to the progression of the nanomedicine field and the protection of pregnant women filling the industry gap of the developmental toxicity risk assessment.

ACKNOWLEDGEMENTS: Project founded by Stiftung ProCare Zurich.

A18. Jorge Sanchez

Phase behaviour of Cellulose nanocrystals doped with melanin and polydopamine

Jorge Sanchez[1], Gilberto Siqueira[2], Gustav Nyström[3]

[1,2,3] *Cellulose and Wood Materials, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

INTRODUCTION: Cellulose nanocrystals (CNC) and similar biopolymers have been thoroughly researched because of their intrinsic ability to form liquid crystalline (LC) phases, especially chiral nematic phases which form structural colours (1). Although several approaches (e.g. introduction of polymeric spacing molecules (2) and metallic nanoparticles (3)) have been envisioned to modify the photonic response (i.e. chiral nematic pitch) of such liquid crystal systems, a persistent challenge remains to modify it via a fully bio-based approach. This would represent a novel step in the development of structurally coloured systems for applications as colour filters in sustainable electronics.

METHODS: The present study investigates the broadband absorption behaviour of custom-made melanin and polydopamine nanoparticles, and their effect on LC tactoid formation (i.e. measuring fingerprint patterns and helicoidal pitch) and phase-separation kinetics (i.e. coexistence of isotropic and anisotropic phases at different time points) of CNC suspensions. This is done to assess the phase behaviour of the combined materials. We also investigate static colour formation in solid state by matching self-assembly conditions for tactoid formation and develop films with a differentiated photonic response.

RESULTS & DISCUSSION: Preliminary results indicate that the photonic response of CNC-based films doped with melanin and polydopamine can be modulated by the addition of less than 0.1 wt.% dopant to 5 wt.% CNC suspensions, followed by the subsequent evaporation of the films, as illustrated in Figure 1.

Fig. 1: *Structurally coloured film samples after evaporation induced self-assembly of doped CNC films.*

CONCLUSIONS: The colour modulation of CNC based systems enables novel materials as components in sustainable electronics, such as translucent colour filters for e-readers, smartwatches, and user interfaces, advancing biodegradable, non-silicon electronics and reducing global e-waste.

ACKNOWLEDGEMENTS: Dr. Gilberto Siqueira, Dr. Gustav Nyström

REFERENCES:

1. Frka-Petesic, B., Parton, T. G., Honorato-Rios, C., Narkevicius, A., Ballu, K., Shen, Q., ... & Vignolini, S. (2023). Structural color from cellulose nanocrystals or chitin nanocrystals: self-assembly, optics, and applications. *Chemical Reviews*, *123*(23), 12595-12756.

2. Andrew, L. J., Walters, C. M., Hamad, W. Y., & MacLachlan, M. J. (2023). Coassembly of cellulose nanocrystals and neutral polymers in iridescent chiral nematic films. *Biomacromolecules*, *24*(2), 896-908.

3. Chen, T., Zhao, Q., Meng, X., Li, Y., Peng, H., Whittaker, A. K., & Zhu, S. (2020). Ultrasensitive magnetic tuning of optical properties of films of cholesteric cellulose nanocrystals. *ACS nano*, *14*(8), 9440-9448.

A19. Suyash Singh

No abstract available.

A20. Jacopo Sorani

Redefining Drug Innovation: How to Integrate the Safe and Sustainable by Design (SSbD) Framework to the Pharmaceuticals and Nanomedicines Sector

Jacopo Sorani, Roland Hischier and Bernd Nowack

Empa, Technology & Society Laboratory, CH-9001 St. Gallen, Switzerland

INTRODUCTION: The pharmaceutical industry has been at the forefront of improving global health but poses environmental risks due to active pharmaceutical ingredients (APIs) entering ecosystems. These compounds, designed to be biologically active, often enter the environment through patient excretion or as a by-product of pharmaceutical production (e.g., Intermediate fine chemicals are pivotal)[1]. For instance, compounds such as 17β-ethinylestradiol can feminize fish at trace levels, and there are over 156 active pharmaceutical ingredients (APIs) found in European waters at concentrations up to 10 µg/L[2]. Ensuring rigorous environmental risk assessment tests and sustainability in production are essential. The Safe and Sustainable by Design (SSbD) framework aims to integrate safety and sustainability early in the development process[3]. This study investigates how SSbD can align with pharmaceutical research and development (R&D) while ensuring safety and efficacy.

METHODS: To assess the integration of the SSbD framework into the drug development process critical phases such as Drug Discovery, Lead Optimization, and Pre-clinical Studies are analyzed[4]. This evaluation focused on the type and availability of existing data, including toxicological and pharmacokinetic profiles, and its potential to support SSbD requirements. Alignment with European regulations, such as GLP, GMP, Directive 2001/83/EC, and Regulation (EC) No. 726/2004, was reviewed to ensure compatibility.

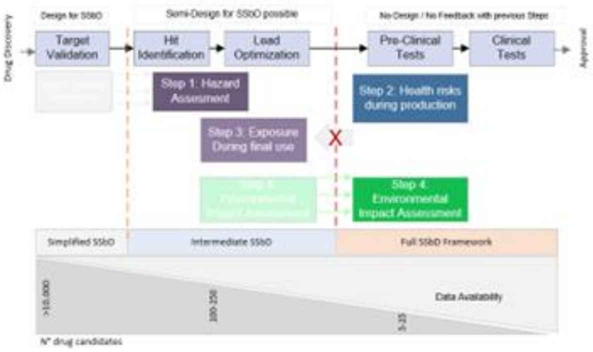


Fig. 1: *How the different steps would be adapted within the drug development process.*

RESULTS & DISCUSSION: Evaluation of three SSbD integration scenarios (simplified, intermediate, and complete) revealed the "intermediate" approach, implemented during lead optimization, as the most feasible. This strategy effectively utilizes existing toxicological and pharmacokinetic data while minimizing disruption to established R&D workflows. Crucially, this approach allows for design adjustments based on sustainability considerations. The study proposes expanding hazard assessments to include antimicrobial resistance and encompass excipients and metabolites. The socio-economical assessment has been expanded, including cost consideration for predicting the cost of overall SSbD based on the characteristics of the substance. Furthermore, the unique challenges of applying SSbD to nanomedicines were addressed, with a focus on the complexity of nanoparticle characterization and testing[5].

CONCLUSIONS: The pharmaceutical sector is predisposed to adopt the SSbD framework due to the extensive data already generated during the drug development process. This enables a seamless integration of sustainability principles, optimizing resource use and minimizing additional testing while maintaining its commitment to safety and efficacy.

REFERENCES:

[1] K. Kümmerer, "The presence of pharmaceuticals in the environment due to human use – present knowledge and future challenges," *J. Environ. Manage.*, vol. 90, no. 8, Art. no. 8, Jun. 2009, doi: 10.1016/j.jenvman.2009.01.023.

[2] J. L. Wilkinson *et al.*, "Pharmaceutical pollution of the world's rivers," *Proc. Natl. Acad. Sci.*, vol. 119, no. 8, Art. no. 8, Feb. 2022, doi: 10.1073/pnas.2113947119.

[3] C. Farcal and G. Aguirre, "Safe and Sustainable by Design chemicals and materials".

[4] A. Deore, J. Dhumane, R. Wagh, and R. Sonawane, "The Stages of Drug Discovery and Development Process," *Asian J. Pharm. Res. Dev.*, vol. 7, pp. 62–67, Dec. 2019, doi: 10.22270/ajprd.v7i6.616.

[5] B. Nowack and T. D. Bucheli, "Occurrence, behavior and effects of nanoparticles in the environment," *Environ. Pollut.*, vol. 150, no. 1, Art. no. 1, Nov. 2007, doi: 10.1016/j.envpol.2007.06.006.

A21. Noé Stauffer

Dynamic optimal model reduction

Noé Stauffer[1,2], Ramzi Dakhmouche[1,3], Hossein Gorji[1], Ivan Lunati[1]

[1] *Computational Engineering, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Scientific Computing and Uncertainty Quantification, EPFL, Lausanne, Switzerland*

[3] *Statistical Field Theory, EPFL, Lausanne, Switzerland*

INTRODUCTION: The Mori-Zwanzig (MZ) formalism[1] provides a rigorous model reduction technique, where only a subset of resolved variables is tracked in time. By virtue of the projection operator, their time evolution is reformulated as a generalized Langevin equation. Its Markovian term depends only on the current value of the resolved variables, the memory depends on the whole history, and the noise term is orthogonal to the projected space and requires the full knowledge of the system. Although formally well defined, the memory integral is the main computational bottleneck of the MZ formalism due its high computational cost. Therefore, the memory integral has been approximated by different approaches. However, there is still lack of flexible and reliable computational treatment, hindering the applicability of the MZ formalism for high-dimensional systems.

METHODS: To tackle this challenge, we opt for a change of perspective by introducing an optimal time-dependent projection operator acting on functions of the Hilbert spaces $\mathcal{H}_t = L^2(R^N, \mu_t)$by taking their μ_t-conditional expectation, given the current state of the chosen resolved variables. Continuously updating the projection operator allows to avoid memory integral effects, as reflected in our pseudo-Markovian integration scheme. In practice however, the probability flow must be known. Following P. Mokrov, A. Korotin et al.[2], we leverage input convex neural networks to learn the probability measure at coarse time steps in an offline stage. The projected dynamic can then be integrated between these updates with fine time resolution by neglecting the memory integral (Fig. 1).

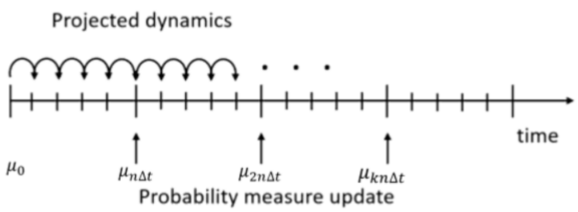


Fig. 1: *Projection operator update strategy: the probability flow* μ_t *is solved at coarse time steps between which the projected dynamics is integrated without memory integral effects.*

RESULTS & DISCUSSION: Focusing on a simple gradient flow, for which the probability flow admits a closed form solution, we show that increasing the number of updates leads to an increased accuracy. Our method outperforms the first order optimal prediction[1].

CONCLUSIONS: The introduced pseudo-Markovian integration scheme leads to a dynamical optimal model reduction technique. Indeed, updating the projection operator allows to avoid memory integral effects. The choice of conditional expectation leads to an optimal projection operator at every update. Moreover, our method is flexible: once the offline computation of the probability flow is performed, our integration scheme can be applied to any function of the state of the system. We aim to extend our method to Hamiltonian flows in future works.

ACKNOWLEDGEMENTS: Funding: Swiss National Science Foundation (grant no. 212876).

REFERENCES:

[1] A. J. Chorin, O. H. Hald, and R. Kupferman. Physica D: Nonlinear Phenomena (2002), 166(3):239–257.

[2] P. Mokrov, A. Korotin, L. Li, A. Genevay, J. Solomon, and E. Burnaev. Large-scale wasserstein gra-dient flows. In Proceedings of the 35th International Conference on Neural Information Processing Systems, NIPS ’21, Red Hook, NY, USA, 2024. Curran Associates Inc.

A22. Akshat Sudheshwar

Approaches to Facilitate Environmentally Safe and Sustainable Decision-Making

Akshat Sudheshwar[1]

[1]*Empa—Swiss Federal Laboratories for Material Science and Technology, Technology and Society Laboratory, St. Gallen, Switzerland*

Keywords: Safe and Sustainable-by-Design (SSbD), Policy Analysis, Methods

This doctoral plan outlines novel Safe- and Sustainable-by-Design (SSbD) methodologies, emphasizing the integration of environmental safety (i.e., hazard, occupational safety and health, and environmental and human risk assessments) with environmental sustainability (impact and lifecycle assessments) at the early stages of innovation. It identifies gaps in current SSbD research, particularly the lack of diverse methods integrating environmental safety and sustainability. Established approaches treat safety and sustainability sequentially rather than concurrently, missing critical trade-offs affecting decision-making. Furthermore, current literature on SSbD lacks a broader policy context, and the links between SSbD and the existing or upcoming environmental legislation in the European Union (EU) remain unclear. Therefore, this research proposal aims to bridge these gaps by proposing methodologies and demonstrating their application through case studies on chemicals, materials, or products.

The primary objective of this doctoral work is to introduce alternative SSbD approaches through tailored methods that simultaneously consider and integrate safety and sustainability criteria. This research plan introduces two primary methodologies: the Probabilistic Multi-perspective Application Selection Approach (pMPAS) and a Multiobjective Optimization Problem (MOOP) approach for SSbD. Furthermore, an in-depth policy analysis of current and upcoming environmental regulations is part of this research plan to understand whether the SSbD framework contributes to better regulatory preparedness.

Overall, the research aims to advance the SSbD field by contextualizing it against environmental policy and developing integrated assessment methodologies that better capture and address the complexities of early-stage innovation and support safer and more sustainable chemical and material development.

A23. Francesco Taddei

Influence of partial curing on residual stress and process time in Additive Manufacturing of thick thermosetting composites

Francesco Taddei*[1,2], Giacomo Struzziero[1], Véronique Michaud[2]

[1] *Laboratory for Mechanical Systems Engineering, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Laboratory for Processing of Advanced Composites, EPFL, Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland*

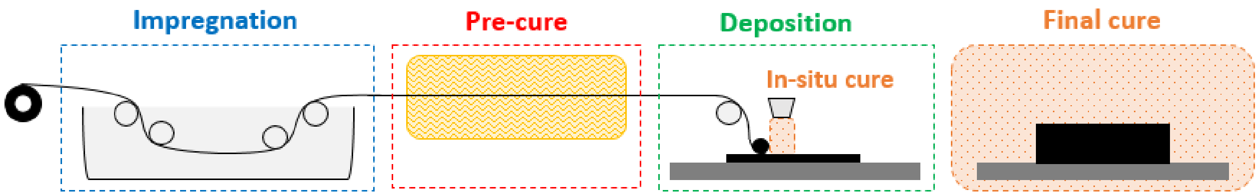


***Fig. 1**: Schematic of the additive process with partial curing.*

INTRODUCTION: Thick section thermosetting composites show significant potential in key industrial sectors; however, their manufacturing poses challenges in terms of process time and arising of process-induced defects. A recent concept for improving manufacturing efficiency and reliability is additive curing, which consists in the additive deposition of impregnated carbon tows while being partially cured through a moving heat source and after they have been possibly pre-cured (Fig. 1).

METHODS: A numerical model of the additive curing process was built in Abaqus to study the effect of pre-cure level, deposition speed, and heat source dimensions and intensity on thermal overshoot, residual stress and process time in the manufacturing of a carbon/epoxy laminate. The resin properties to feed the model were characterised as a function of cure degree and temperature. Strain monitoring during cure was performed using optical fibres for validation purposes.

RESULTS & DISCUSSION: The partial curing strategy can mitigate temperature overshoot, residual stress, and stress gradient during cure by up to 92%, 20% and 65%, respectively, compared to standard curing. Total process time is decreased by 23%. However, since the thermal overshoot might speed up the reaction, optimal process parameters may target the shortest process time while keeping defects within acceptable levels.

CONCLUSIONS: This study explores the possibilities of additive curing aiming at opening new design opportunities for a reliable and efficient manufacturing. Future studies should investigate when this process is convenient and its limits before it can potentially be scaled up and strongly change how composite components are produced.

ACKNOWLEDGEMENTS: This work was supported by the Laboratory for Mechanical Systems Engineering, Swiss Federal Laboratories for Materials Science and technology (Empa) through the Empa Board of Directors. Valentin Ott, Cyrill Schmid and Dr. Michel Barbezat are kindly acknowledged for the technical support in the experimental activities.

REFERENCES:

[1] T.A. Bogetti, J.W. Gillespie, Process induced stress and deformation in thick section thermoset composite laminates, J. Compos. Mater. 26(5):626-660, 1992.

[2] G. Struzziero, M. Barbezat, A.A. Skordos, Assessment of the benefits of 3D printing of advanced thermosetting composites using process simulation and numerical optimization, Addit. Manuf. 63:103417, 2023.

[3] F. Taddei, M. Barbezat, E. Troiani, G. Struzziero, Influence of pre curing stage in additive manufacturing of advanced thermosetting composites, In European Conference on Composite Materials ECCM20, 2022.

[4] P. I. Karkanas and I. K. Partridge, Cure modeling and monitoring of epoxy/amine resin systems. I. Cure kinetics modelling, J. Appl. Polym. Sci. 77(7):1419-1431, 2000.

[5] M. Sadeghinia, K. M. B. Jansen and L. J. Ernst, Characterization and modeling the thermo-mechanical cure-dependent properties of epoxy molding compound, Int. J. Adhes. Adhes. 32:82-88, 2012.

[6] J.T. Tsai, J.S. Dustin, J.A. Mansson, Cure strain monitoring in composite laminates with distributed optical sensor, Compos. Part A-Appl. S. 125:105503, 2019.

[7] N. An, G.Y. Yang, K. Yang, J. Wang, M.E. Li, J.X. Zhou, Implementation of Abaqus user subroutines and plugin for thermal analysis of powder-bed electron-beam-melting additive manufacturing process, Mater. Today Commun. 21:102307, 2021.

A24. Umut Taylan

Fabrication of Sub-10 µm Size Asymmetric Microstructures by Mask Projection Laser Ablation with Gray Level Transmission Intensities

Umut Taylan[1], Benjamin Minnig[1], Nicolas Zaugg[1], Patrik Hoffmann[1]

[1]*Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Advanced Materials Processing, Thun, Switzerland*

The precise fabrication of sub-10 µm asymmetric microstructures is critical for applications like gravure printing but it remains a significant challenge due to substrate variability and the need for fine optical control. This research explores mask projection laser ablation method by using grayscale transmission masks to create micrometric 2.5D structures on polycarbonate substrates over large areas. A 248 nm nanosecond KrF excimer laser with fluences below 1 J/cm² was employed, combined with a floating objective head to overcome substrate thickness variations. The grayscale masks modulate light transmission, enabling controlled material ablation and the generation of curved walled microstructures through the incubation effect.

Results show that 8×8 µm asymmetric microstructures are successfully fabricated, as validated through SEM imaging. Furthermore, differences in transmission intensities were demonstrated to influence ablation rates and depth profiles, allowing the successful fabrication of diverse microstructure geometries. These findings highlight the importance of optimizing both process parameters and mask designs for precision outcomes.

This work paves the way for scalable industrial applications, such as gravure cylinder engraving for functional printing at speeds up to 1 m/s in SCALAR project. Future efforts aim to refine the optical transfer function of the laser system, enabling even more precise microstructuring. By overcoming challenges in substrate variability and scaling, this research contributes to advancing high-speed, functional printing technologies, potentially revolutionizing the field of advanced manufacturing.

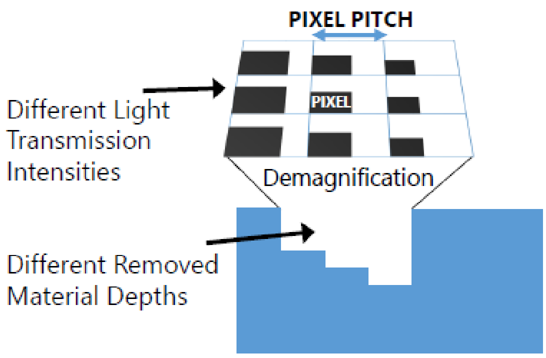


Figure 1: *Concept of grayscale mask in mask projection laser ablation method*

A25. Alex Weitnauer

Airborne mid-infrared spectroscopy for in-situ water vapor isotope measurements in the upper atmosphere

Alex Weitnauer[1, 2], Lorenz Heilmann[1], Lukas Emmenegger[1], and Béla Tuzson[1]

[1] *Empa – Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Air Pollution/Environmental Technology, 8600 Dübendorf, Switzerland*

[2] *Institute for Atmospheric and Climate Science, ETH Zürich, 8092 Zürich, Switzerland*

Water vapor is the main greenhouse gas controlling the Earth’s energy balance particularly in the upper troposphere and lower stratosphere (UTLS). Monitoring its variability in the UTLS is crucial for understanding the climate system but lacks important information about the history and the origin of the water vapor.

Here, water isotopologues have the potential to answer open questions concerning the atmospheric water vapor budget since the distribution of isotopes in the different phases depend on environmental conditions, making stable water isotopes ($H_2{}^{16}O$, $H_2{}^{18}O$, and HDO) an ideal proxy for process studies of the hydrological cycle. Despite the large potential of such measurements, the availability of in-situ data is still quite limited due to a lack of adequate analytical tools.

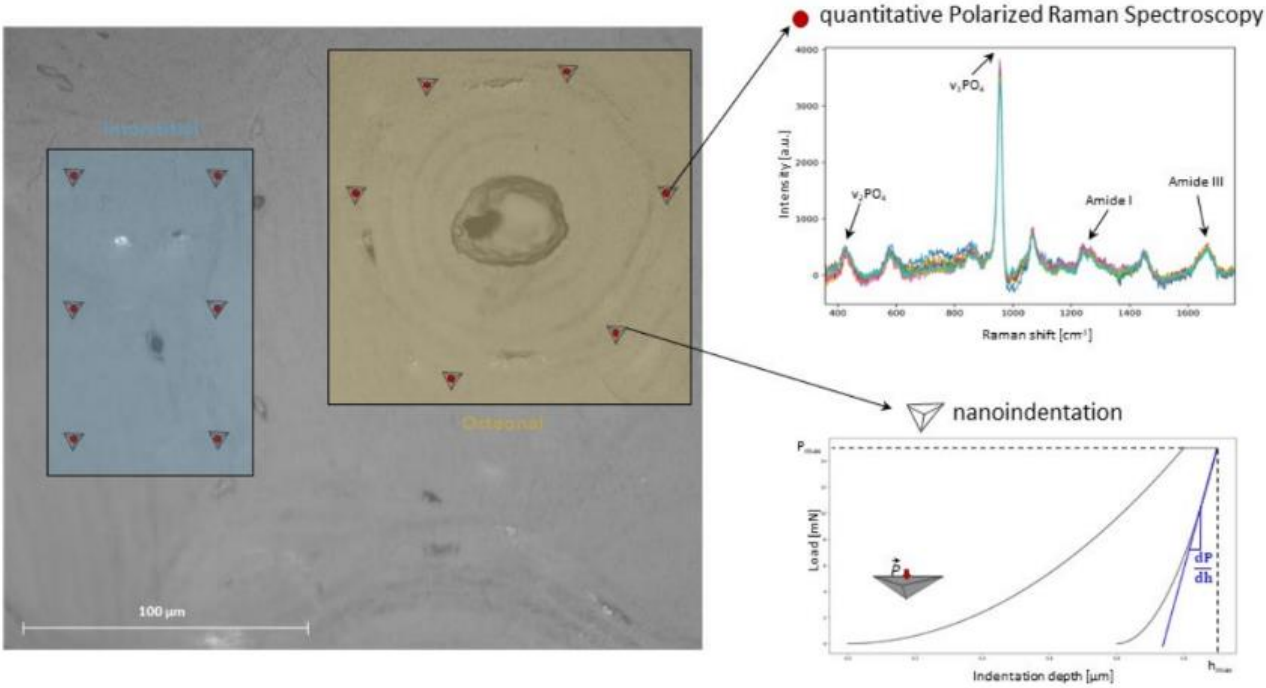
This project focuses on the development of a mobile laser spectrometer targeting airborne in-situ measurements of water isotopologues in the upper atmosphere. A selected quantum cascade laser (QCL) (≈ 7 µm) enables the interrogation of the strong absorption features of water molecules in the mid-infrared region.

The low abundance of the rare water vapor isotopologues has to be compensated by substantially extending the optical path length (OPL) (>250 m), and thereby, improving the signal-to-noise ratio (SNR). This requires a reconception of multi-pass cells (MPC) which enables efficient folding of the laser beam into a compact volume and assures rigidity needed for harsh environmental conditions.

Ultimately, the aim is to provide an easy-to-deploy tool for isotope-resolved water vapor profiles at high spatio-temporal resolution.

A26. Valeria Zanrè

Influence of osteoporosis and COVID-19 on bone microscale properties: A Raman spectroscopy and nanoindentation study



Bone fragility, often associated with osteoporosis, represents a significant global socioeconomic burden. Emerging evidence of COVID-19's long-term impact on multiple organ systems, alongside recent findings of bone loss during the acute phase of infection, raises concerns about increased fracture risk, especially for populations already at higher risk of skeletal health issues. Traditional methods for assessing fracture risk, such as bone mineral density (BMD) measurements, are limited by high error margins. This underscores that bone strength is influenced by bone quality factors beyond BMD, such as microscale compositional and mechanical properties.

This study analyzed 23 cortical bone samples from femoral neck biopsies of postmenopausal women undergoing hip arthroplasty, classified as healthy, osteoporotic, or having had COVID-19 within 12 months. Microscale compositional and mechanical properties were assessed using site-matched nanoindentation testing and quantitative polarized Raman spectroscopy. Multivariate analyses using mixed-effects models revealed significant trends: osteoporotic and COVID-19 samples exhibited reduced matrix maturity ratios (-3.52% and -4.47%, respectively) and increased crystallinity (1.31% and 1.25%, respectively). While only osteoporotic samples showed significantly reduced hardness, both conditions amplified the mineral-to-matrix ratio's effects on micromechanical properties, suggesting potential pathophysiological changes in mineral and matrix balance linked to bone loss. An optimized model accurately predicted Young's modulus and hardness (R^2: 66–70%; Lin's concordance: 0.75–0.81) without overfitting.

The methodology demonstrated in this study shows promise for detecting pathological bone conditions and offering valuable insights into disease-induced microscale alterations, laying the groundwork for improved diagnostic tools, advanced modeling techniques, and innovative treatment strategies to improve patient care.

A27. Cansu Zeytun Karaman

ETHYLSULFONE-CONTAINING POLYSILOXANES FOR DIELECTRIC ELASTOMER ACTUATORS

Cansu Zeytun Karaman, Thulasinath Raman Venkatesan, Frank Nüesch, Dorina M. Opris

Dielectric elastomer actuators (DEAs) are versatile soft transducers with significant potential in various applications, particularly in the fields of soft robotics, energy harvesting, and adaptive systems. These devices function by utilizing a dielectric elastomer film placed between two stretchable electrodes. When an electric field is applied, the film undergoes deformation, enabling the generation of force and mechanical motion. To achieve enhanced performance, multiple DEAs can be combined in a layered configuration to form a stack actuator, which increases the overall force output while maintaining flexibility and adaptability. In this study, a novel class of polysiloxanes functionalized with ethylsulfone groups was developed to address the limitations of conventional dielectric elastomers. The introduction of this functional group significantly enhanced the dielectric permittivity of the materials, which is a key parameter for efficient actuation. Additionally, the incorporation of butanethiol in varying proportions allowed precise tuning of the electromechanical properties, including dielectric and mechanical performance. By optimizing the composition, the resulting elastomer exhibited outstanding properties, such as a high dielectric permittivity of 19.42 at 10 kHz (measured at 25°C), combined with a low electrical conductivity. These characteristics contributed to its ability to achieve a large actuation strain of 13.9% at a low electric field of 8.18 V/µm (1 Hz, 900 V).

The material's performance was further evaluated through the construction of a stack actuator comprising five dielectric layers. This multilayer device demonstrated a thickness strain of 3.3% under an electric field of 14.5 V/µm at 1 Hz (1600 V), showcasing its ability to deliver significant mechanical displacement under practical operating conditions. The stack actuator also exhibited stable actuation across a range of frequencies, including 5 Hz and 10 Hz at an applied voltage of 1200 V. Notably, at 1.00 Hz, the actuator maintained consistent performance over 2000 cycles, indicating excellent operational stability and durability.

A28. Wolfgang Jan Zucha

EFFECT OF MAGNESIUM-BASED CEMENTITIOUS BINDER ON SMECTITE FOR EARTH CONSTRUCTION

Wolfgang Jan Zucha[1/2], Raphel Kuhn[2], Michael Plötze[1], Ellina Bernard[2]

[1] *ClayLab, ETH, Zurich, Switzerland*

[2] *Concrete & Asphalt Group, Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, Switzerland*

To achieve carbon-neutral construction, (sub)soils used as earth concrete offer a promising solution [1]. Soils are infinitely recyclable and do not require energy-intensive processing. However, adding a cementitious-based binder is still necessary because dried soils do not exhibit the same strength as concrete. Additionally, soils with a high content of the clay mineral "smectite" are unsuitable for construction due to their shrinkage and cracking upon drying [1] In this study, a potential solution is presented: Magnesium-based cementitious binder (MB), which is produced with a low-to-negative CO2 emission [2]. Different bentonites were mixed with MB and characterised at different curing times. Results show that adding MB transforms smectite into a chlorite-like clay mineral within hours. This newly formed clay mineral is known as hydroxy-interlayered smectite (HIS). In a HIS, the smectite interlayer is exchanged by oligomeric Mg-hydroxyl. Compared to common smectite, HIS has strongly reduced cation exchange capacity, reduced specific surface area, and, most important, reduced swelling and shrinkage capacity. Therefore, MB has the advantage to stabilise smectite-rich soils as a cement, and additionally reduce the shrinkage by altering the fundamental properties of smectite (Figure 1). Furthermore, this study shows a simpler method to transform smectite into HIS than in previous studies, e.g. [3], and its constraints.

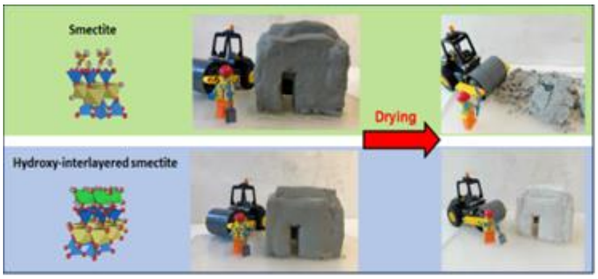


Figure 1: *Comparison of a "clay-house" made of smectite and hydroxyl-interlayred smectite (HIS) before and after drying.*

REFERENCES:

[1] H. Van Damme and H. Houben, "Earth concrete. Stabilization revisited," *Cem. Concr. Res.*, vol. 114, pp. 90–102, 2018, doi: 10.1016/j.cemconres.2017.02.035.

[2] E. Bernard *et al.*, "MgO-based cements – Current status and opportunities," *RILEM Tech. Lett.*, vol. 8, pp. 65–78, 2023, doi: 10.21809/rilemtechlett.2023.177.

[3] G. S. Xeidakis, "Stabilization of swelling clays by Mg(OH)2. Factors affecting hydroxy-Mg-interlayering in swelling clays," *Eng. Geol.*, vol. 44, no. 1–4, pp. 93–106, 1996, doi: 10.1016/s0013-7952(96)00046-4.

B1. Raluca-Ana-Maria Barna

The Ligamentum Flavum's Role in Spine Degeneration and Aging

<u>Raluca-Ana-Maria Barna[1,2,3]</u>, Jonas Widmer[3,4], Ameet K. Aiyangar[5,6], Annapaola Parrilli[1]

[1] *Center for X-Ray Analytics Empa, Dübendorf, Switzerland*

[2] *University of Bern, Bern, Switzerland*

[3] *Spine Biomechanics, Balgrist University Hospital, Zurich, Switzerland*

[4] *Department of Orthopedics, Balgrist University Hospital, Zurich, Switzerland*

[5] *D.I.P.R., Insel, Bern; Medizinische Fakultät, Uni Bern*

[6] *Mechanical Systems Engineering, Empa, Dübendorf, Switzerland*

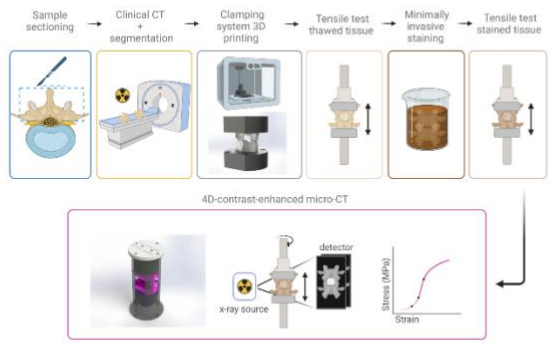


*Figure 1: **Schematic illustration of the materials and methods applied in this study.** Sample processing steps from sample preparation, set up design, and mechanical-structural analysis.*

INTRODUCTION: Lumbar spinal stenosis, the narrowing of the spinal canal causing lumbosacral nerve compression, leads to low back pain and leg symptoms, affecting 5 in 100,000 people annually (1). The compression often results from the enlargement of the ligamentum flavum (LF) (2), which is in close contact with the spinal canal. In patients with LSS, the morphology and function of the LF are altered, as shown by 2D histological studies (3,4). Biomechanical studies have also shown degeneration-related decreases in the stiffness and ultimate strength of the LF, which compromise the stability of the spinal segment (5).

To date, the LF's histology and microstructure have been studied only with 2D imaging. A detailed 3D analysis of its structure and biomechanics could enhance understanding of the condition's pathophysiology and guide new treatments. This project aims to correlate 3D structural and histological changes in the LF with biomechanical and clinical factors using advanced X-ray staining and 4D-contrast-enhanced micro-CT.

METHODS: First, the non-destructive biomechanical and imaging investigation will be performed on the LFs of healthy donors. The ligament will be subject to a tensile test with an in-house designed and sample-specific 3D-printed clamping system, before and after the x-ray staining procedure. Subsequently, the ligament will undergo in situ mechanical loading combined with 3D microstructural visualization.

In the second step, the pathological ligament biopsies undergo a high-resolution structural analysis, aiming to transpose the correlation individuated for the healthy specimens between 3D histomorphology and biomechanics to the pathological samples.

ACKNOWLEDGEMENTS: The project is supported by Empa the Zukunftsfonds. We are grateful to M. Suter for the technical support in the collection of clinical samples.

REFERENCES:

(1) Siebert E. et al. Nat Rev Neurol 5 (2009)

(2) Ciricillo SF. et al. West J Med (1993)

(3) Schräder P. et al. E Spine J 8 (1999).

(4) Jain M. et al. World J Orthop. (2022)

(5) Cornaz F. et al. The Spine Journal. (2014)

B2. Martina Birocco

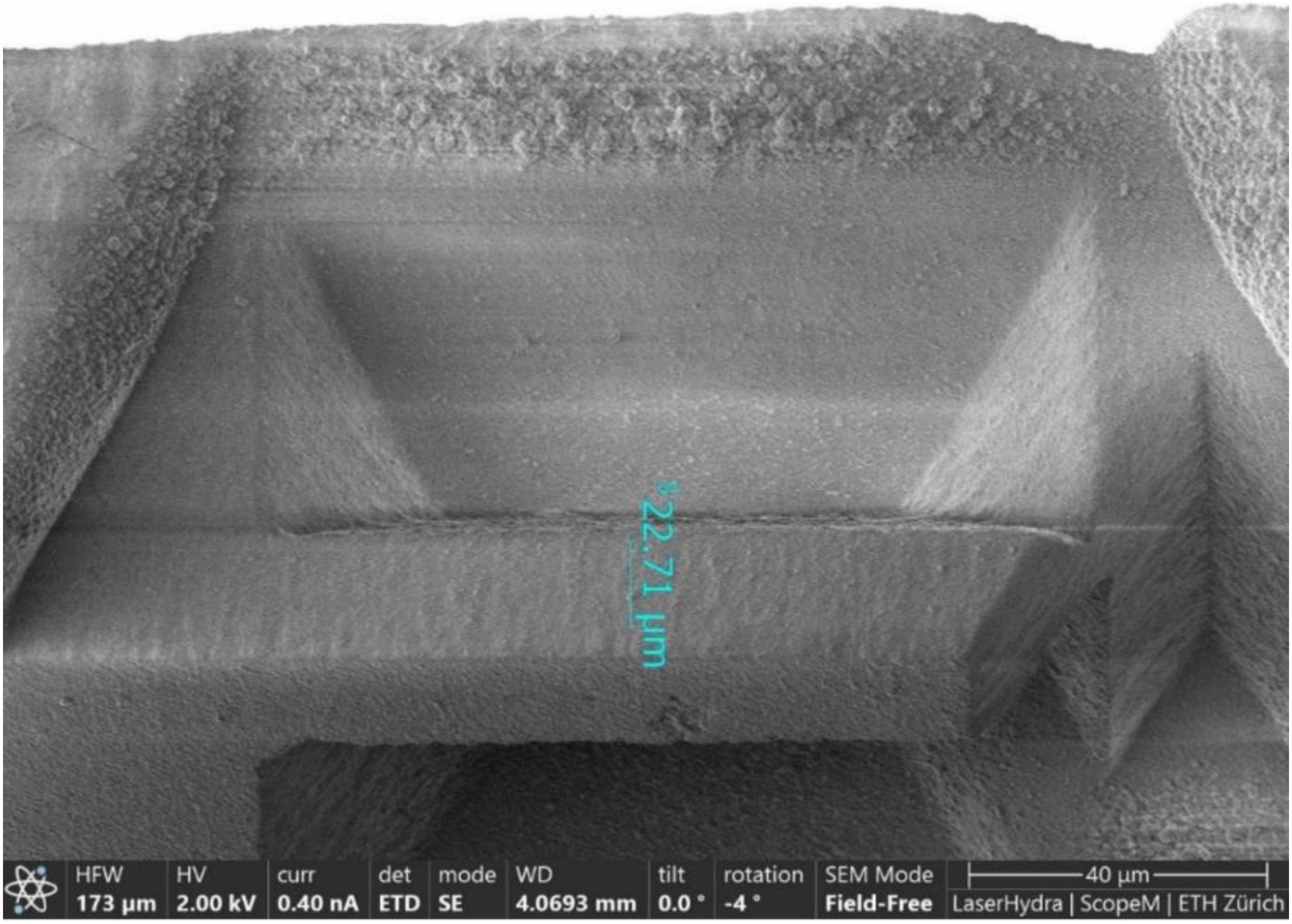


***Figure 1.** Laser ablated cantilever beam*.

Slow crack growth (SCG) is a critical phenomenon in ceramics, where cracks propagate slowly over time, even under stress levels below the material's nominal strength, often leading to catastrophic failure. SCG is influenced by environmental humidity, which can weaken atomic bonds at the crack tip, accelerating crack propagation. Understanding SCG is crucial for ensuring the long-term reliability of ceramics.

Recent studies have explored this phenomenon at the microscale, but they have been limited in terms of the environmental conditions tested. This study aims to investigate alumina's fracture behavior under a broad range of humidity levels and develop a model its performances across varying environmental conditions.

Mono- and polycrystalline alumina samples were machined into cantilever beams using laser ablation and tested with a nanoindenter under varying humidity and loading conditions. FEM models were employed to analyze the crack propagation mechanism within the sample during SCG. A Bayesian regression process was applied to model the relationship between stress intensity factors and humidity in the testing environment.

Preliminary results show that fracture toughness decreases with increasing humidity, but not linearly. The fracture intensity factor declines more rapidly at lower humidity levels, stabilizing around 75%, probably due to saturation of water molecules interacting with atomic bonds at the crack tip.

This study offers a comprehensive understanding of alumina's performances in terms of fracture toughness under different environmental conditions, also introducing a promising approach to studying SCG at the microscale on various materials, providing greater accuracy and significantly faster results compared to previously used methods.

B3. Sofiia Butenko

3D-printed composites with aligned 1D lead-free piezoelectric ceramic fillers for soft self-powered tactile sensors for soft grippers

Sofiia Butenko, Arun Ichangi, and Frank Clemens*

Laboratory for High Performance Ceramics, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

Motivation: Soft grippers are gaining popularity due to their simple control systems and safe handling of diverse-shaped objects. To achieve close-loop control, implementation of sensing capabilities is required. This can be addressed by the development of soft sensing composites made from elastomers matrix materials with embedded piezoelectric ceramic fillers, and their structural integration into the soft gripper design. This innovation will enable the production of functional grippers with broader capabilities to boost their industrial robotization.

Problem statement: To have the task diversity, the tactile sensor for soft grippers should possess high sensitivity, low energy consumption, fast response time, and softness. Existing tactile sensors demonstrate energy consumption while maintaining the necessary softness. In this work, we aim to develop a composite material by aligning piezoceramic fibers to achieve a soft self-powered tactile sensor.

Planned approach: We will create a composite material by embedding lead-free barium titanate ($BaTiO_3$, BTO) and potassium sodium niobate (KNN, $(K,Na)NbO_3$) piezoceramic fibres into thermoset elastomers. Therefore, we synthesize BTO and KNN fibres and conducting a thorough characterization of their properties. In the next step, we embed and align these fibres into the elastomer matrix using a dielectrophoresis process. We aim to understand how the nature of the elastomer, applied voltage, fibres shape, and sample thickness influence the alignment process. The final goal is to integrate the aligning process into a 3D printing process to be able to print different design structures of the self-powered tactile sensor composite material. These structures will be integrated in a soft gripper demonstator to determine their suitability for use in soft-robotic tactile sensor applications.

Acknowledgements: The authors gratefully acknowledge the financial support of Swiss National Science Foundation (SNSF).

B4. Vahid Charkhesht

The Effect of Graphene on Fast Charging and Discharging Performance of LFP in Li-Ion-Based Supercapacitors

Keywords: Graphene, Lithium Iron Phosphate (LFP), Li-Ion Supercapacitors, Fast Charging, Electrochemical Performance, Energy Storage

With the increasing demand for high-performance energy storage systems, lithium-ion-based supercapacitors (Li-ion SCs) have gained significant attention due to their high-power density, fast charge-discharge capabilities, and long cycle life. However, improving the rate performance and energy density remains a challenge, particularly in lithium iron phosphate ($LiFePO_4$, LFP)-based systems. This study investigates the impact of graphene as a conductive additive in LFP cathodes to enhance charge transport, reduce internal resistance, and improve the electrochemical performance of Li-ion SCs. The incorporation of graphene into the LFP matrix is expected to enhance electron mobility, facilitate rapid ion diffusion, and improve structural stability under high-power cycling conditions. The results indicate that the graphene-modified LFP exhibits superior fast-charging behavior, higher capacitance retention, and reduced charge transfer resistance compared to conventional LFP-based electrodes. These findings demonstrate the potential of graphene as a key material for optimizing LFP-based supercapacitors for high-power applications such as electric vehicles and renewable energy storage systems.

B5. Shungui Deng

Insights into the Overcharge-Induced Failure Mechanism of Lithium-Sulfur Batteries

Shungui Deng[1,2], Chuanfang (John) Zhang [3], Frank Nüesch[1,2], Jakob Heier[1]

[1]*Empa, Swiss Federal Laboratories of Materials Science and Technology, Switzerland*

[2] *Institute of Materials Science and Engineering, Ecole Polytechnique Federale de Lausanne (EPFL), Station 12, Lausanne, CH-1015 Switzerland*

[3] *College of Materials Science & Engineering, Sichuan University, Chengdu, 610065, Sichuan, China*

Lithium sulfur (Li-S) batteries, known for their high theoretical energy densities, are regarded as next generation energy storage technology.[1] Besides the well-known "shuttle effect" causing capacity diminution, Li-S batteries also suffer from random overcharging failures during charging phase, marked by sudden drops and fluctuations in voltage-capacity profile (Figure 1).

Here, we systematically investigates the overcharging failure and its underlying mechanisms. Experimental results reveal failure comes from a soft internal short-circuit (ISC) caused by excessive lithium dendrite growth (Figure 1). And we identify the sulfur cathode as the primary driver of this dendrite growth rather than the lithium anode.

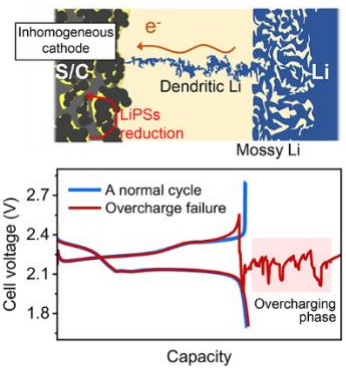


Figure 1: *Overcharging phenomena and processes in a charging-discharging cycle.*

We analyzed the electrochemical processes during the overcharging phase, and also identified the generation of a by-product. By analyzing the structural properties of sulfur cathode such as topography and pore connectivity, and through combined experiments and theoretical simulations, we uncovered the complex mechanisms by which the cathode influences lithium dendrite growth. Finally, we also propose an effective "interlayer" strategy to mitigate above overcharging failure.

References:

[1] 1 S. G. Deng, T. Z. Guo, J. Heier, C. F. Zhang, Advanced Science 2023, 10, 5, 2204930.

B6. João Pedro Ferreira Assunção

SQUARAINE DYE BASED ORGANIC PHOTOMULTIPLICATION DIODES WITH 220% EXTERNAL QUANTUM EFFICIENCY AT 1240 NM

João Pedro Ferreira Assunção[1,2], Elodi Didier[1,3], Joshua Csucker[1], Michael Bouer[1], Roland Hany[1]*, Frank Nüesch[1,2]

[1] Functional Polymers, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

[2] Institute of Materials Science and Engineering, Ecole Polytechnique Fédérale de Lausanne, EPFL, Station 12, CH-1015 Lausanne, Switzerland.

[3] Institute of Chemistry and Chemical Engineering, Ecole Polytechnique Fédérale de Lausanne, EPFL, Station 12, CH-1015 Lausanne, Switzerland.

INTRODUCTION: Near-infrared (NIR) light detection at wavelengths λ > 1100 nm enable broad applications in the medical field. Despite the potential application, NIR organic photodetectors (OPDs) suffers from a lack of available organic dyes with peak absorption beyond the silicon bandgap. Here, a novel NIR squaraine dye was used to fabricate photomultiplication OPDs with peak sensitivity beyond 1100 nm.

METHODS: Photomultiplication OPDs were fabricated by coating TiO2 on ITO, followed by NiO layer deposited by RF sputtering at room temperature. The active layer, 3% wt squaraine dye (RSQ2, Fig 1b, insert) mixed into a PCBM matrix, was spin coated. Lastly BCP, TPBi and Al were thermally evaporatedas electrodes. The architecture is shown in (Fig. 1 a).

RESULTS & DISCUSSION: The OPD achieved an external quantum efficiency (EQE) of 220% at 1240 nm while maintaining 25% in the absorption tail at 1400 nm, thereby surpassing existing NIR OPDs by a factor of 10 (Fig. 1b)[1]. The measured maximum total Noise is 10^9 Jones at 1240 nm, and the detectivity estimated from the shot noise is ≈1011 Jones, independent of the bias voltage.

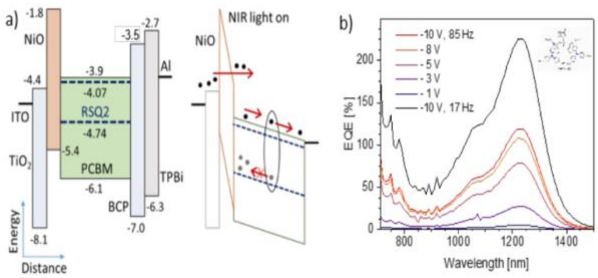


***Fig. 1:** a) OPD stack indicated energy values and the operation process. b) EQE spectra at different voltages and chopper frequencies.*

CONCLUSIONS: RSQ2 was applied in NIR OPD reaching 10x higher EQE than previously reported OPDs. Since organic devices can be flexible and low cost. This represents a step forward to health monitoring and treatment wearable devices.

ACKNOWLEDGEMENTS: Financial support from the SNF (Grant No. CRSII5_216629/1) is acknowledged.

REFERENCES:

[1]I. Park, Adv. Opt. Mater. 10 (2022) 1–8.

B7. Corentin Foucher

Multiscale investigation of impact mitigation strategies: Biomimicking musk ox head

Corentin Foucher, Dr Jakob Schwiedrzik, Prof. Dr. Johann Michler

[1] *Laboratory for High Performance Ceramics (201), Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

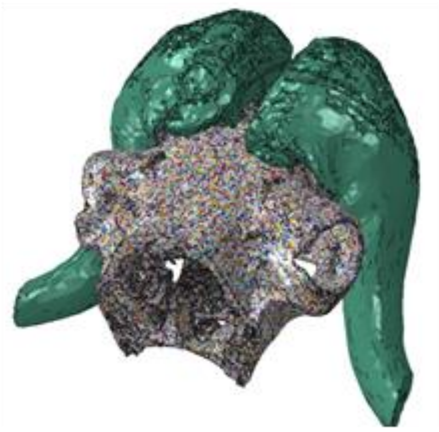


Fig. 1: Macroscale finite element model of the muskox skull. Colors indicate variations in material properties. Each element in the bone region is assigned properties calculated based on the bone density observed in CT scans.

INTRODUCTION: The muskox (Ovibos moschatus), a member of the Bovidae family, evolved to survive harsh Arctic conditions during the Pleistocene. Among its notable behaviors is the repeated head-first ramming during intra-species clashes by male specimens reaching weights of up to 400 kg and speeds of 40 km/h. Despite the extreme forces involved, the muskox skull demonstrates remarkable impact resistance, suggesting evolutionary adaptations optimized for high-energy absorption and stress distribution.

This research aims to investigate the unique structural characteristics of the muskox skull to develop bioinspired mechanical metamaterials capable of mitigating repeated impacts without relying on plastic deformation or allowing crack propagation.

METHODS: CT scans give data on the bone's internal structure on a macroscopic scale. Using these 3D volumes to construct a Finite Element Model of an impact on the skull, enables us to study the mechanisms at play in this animal's skull during impact. Adopting a multiscale approach, the study combines imaging data at varying resolutions to account for the effects of both macroscale structures and trabecular microstructures.

RESULTS & DISCUSSION: Initial macroscale analyses reveal several mode shapes that can be excited by an impact to the top of the skull. Notably, nodal points—regions with minimal movement—are located near the brain cavity, suggesting a natural protective mechanism that minimizes strain and energy transfer to the brain.

CONCLUSIONS: By mimicking these natural mechanisms, the project seeks to design novel metamaterials with applications in fields requiring lightweight, high-performance impact-resistant materials, such as aerospace, automotive safety, and protective gear.

REFERENCES:

[1] Drake A. et al., "Horn and horn core trabecular bone of bighorn sheep rams absorbs impact energy," Acta Biomaterialia, 2016.

[2] Aguirre TG et al. Bioinspired material architectures from bighorn sheep, Sci Rep, 2020.

B8. Stefanie Frick

Accelerating the development of oxynitride coatings using combinatorial magnetron sputtering

Stefanie Frick[1], Oleksandr Pshyk[1], Alexander Wieczorek[1], Kerstin Thorwarth[1], Arnold Müller[2], Sebastian Siol[1]

[1] Laboratory of Surface Science & Coating Technologies, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

[2] Laboratory of Ion Beam Physics, ETH Zurich, Zürich, Switzerland

INTRODUCTION: Oxynitrides are a class of materials with applications including photocatalysts, phosphors, pigments, wear resistant coatings or high k-dielectrics [1,2]. This wide range of applications is made possible in particular by the tunability of their optical, electrical and mechanical properties by varying their anion stoichiometry. Combinatorial magnetron sputtering is a commonly applied technique to rapidly screen the compositional dependence of properties of interest. In the literature, this is mostly limited to sputtering cation gradients on a substrate, whereas additional anion gradients would be very useful for screening oxynitride systems.

METHODS: Three different approaches to obtaining orthogonal anion and cation gradients by magnetron co-sputtering were investigated, including different locations of the reactive gas inlets and different target material combinations. The Al-Si-O-N system was chosen for this proof of concept, as it is of interest for protective transparent coatings with variable refractive indices [3,4].

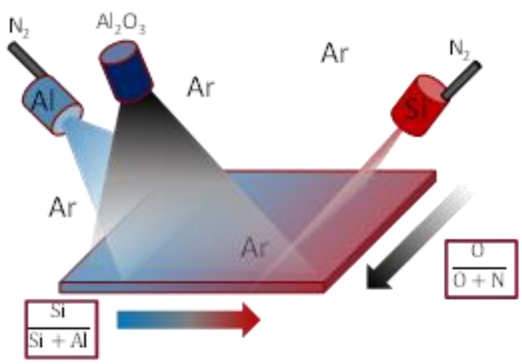


Fig. 1: *Reactive magnetron sputtering configuration to obtain controllable, orthogonal anion and cation gradients.*

RESULTS & DISCUSSION: Applying the most promising approach, an anion spread of 1-45% O/(N+O) and a cation spread of 5-40% Si/(Al+Si) was achieved within only 5 deposition runs. The corresponding mechanical and optical property mapping showed a maximum hardness of 23-24 GPa at low Si and O contents, while the refractive index varied from 1.80-2.02 with decreasing oxygen anion content.

CONCLUSIONS: The results presented encourage the application of this two-dimensional composition screening approach to other promising quaternary oxynitride systems, which should accelerate the custom co-optimisation of properties as required for (multi)functional coatings in industrial applications.

REFERENCES:

[1] F. Vaz, N. Martin, M. Fenker, Eds., Metallic Oxynitride Thin Films by Reactive Sputtering and Related Deposition Methods: Process, Properties and Applications, Bentham Science Publisher, 2013.

[2] R. J. Xie, H. T. Hintzen, J. Am. Ceram. Soc. 96 (2013) 665–687.

[3] A. Pélisson et al., Surface and Coatings Technology 202 (2007) 884-889.

[4] M. R. Fischer et al., Science and Technology of Advanced Materials 20 (2019) 1031-1042.

B9. Sebastian Habermann

Cathodoluminescent and Characteristic X-ray-emissive Rare-Earth-doped Core/Shell Protein Labels for Spectromicroscopic Analysis of Cell Surface Receptors

Sebastian Habermann[1, 2], Lukas R. H. Gerken[1, 2], Mathieu Kociak[3], Christian Monachon[4], Vera M. Kissling[2], Alexander Gogos[1, 2] and Inge K. Herrmann[1, 2, 5, 6]

[1] Nanoparticle Systems Engineering Laboratory, Institute of Energy and Process Engineering, Department of Mechanical and Process Engineering, ETH Zurich, Sonneggstrasse 3, 8092 Zurich, Switzerland.

[2] Laboratory for Particles Biology Interactions, Department Materials Meet Life, Swiss Federal Laboratories for Materials Science and Technology (Empa), Lerchenfeldstrasse 5, 9014 St. Gallen, Switzerland.

[3] Université Paris-Saclay, CNRS, Laboratoire de Physique des Solides, Orsay 91405, France.

[4] Attolight AG, Chemin de la Venoge 11, 1024 Ecublens, Switzerland.

[5] The Ingenuity Lab, University Hospital Balgrist, Balgrist Campus, Forchstrasse 340, 8008 Zurich, Switzerland.

[6] Faculty of Medicine, University of Zurich, Rämistrasse 74, 8006 Zurich, Switzerland.

Microscopy has been pivotal for our understanding of fundamental biological processes by unveiling previously unattainable scales. However, understanding nanoscale interactions of biomolecules and intertwining them in a cellular context remains a major challenge as light diffraction events limit the achievable resolutions. Electron microscopy (EM), unlike light-based techniques, provides access to the cellular ultrastructure but results in grayscale images, preventing unambiguous (co-)localization of targets without tracers or correlative approaches.

This study introduces nanoparticle-based protein labels for correlative cathodoluminescence electron microscopy (CCLEM) and energy-dispersive X-ray spectromicroscopy (EDX-SM). By incorporating rare-earth dopants in a low phonon host lattice and shielding them from non-radiative quenching with an inert shell, the characteristic cathodoluminescence (CL) and X-ray emissivity of sub-20 nm nanoparticles were utilized as unique spectral fingerprints for precise label localization and identification. The core/shell nanoparticles were functionalized with either folic acid (terbium-doped) or caffeic acid (europium-doped), linking the single-particle response to a biological entity. Their protein-labeling potential was examined using HeLa cells expressing different surface receptors that bind to folic or caffeic acid, respectively.

Single-particle cathodoluminescence, along with a distinctive energy-dispersive X-ray signature, was successfully demonstrated for both populations, with the latter outperforming CL as a response for ColorEM. EDX-SM impressed with swift imaging times well below 2 minutes per µm² while offering high resolution with a pixel size of 2.78 nm, enabling the observation of biologically relevant areas.

These results pave the way for multi-color labeling based on electron spectromicroscopy and show its potential for studying innovation-bearing structure-function relationships at the protein level.

B10. Mohammad Jafarpour

Impact of Cavity Parameters on Gravure Printing for Printed Electronics

Mohammad Jafarpour

Gravure printing, renowned for its exceptional speed and high-resolution output, has long been a cornerstone technology in the graphics and art industries. Economical mass production in these fields benefits from the fact that defects as small as 10 µm are invisible to the human eye and can be disregarded. However, in printed electronics, even minor defects can lead to malfunctions in the final device. Accurate ink transfer on a micrometer scale is, therefore, crucial for printed electronics. Ink transfer is a complex, nonlinear process, where the shape of the gravure cylinder cavities plays a critical role in facilitating filling, wiping, and the transfer of ink from the cavity to the substrate.

Within the Strategic Focus Area Advanced Manufacturing project of the ETH domain, the SCALAR consortium—comprising five ETH-domain research groups and four industry partners—proposes a novel cylinder engraving process that enhances resolution and allows greater freedom in cavity shape design. In this study, we employed laser ablation to engrave cavities into polycarbonate (PC) film, followed by pattern transfer into a nickel (Ni) shim via electroplating. This Ni shim was subsequently laminated onto a gravure plate or cylinder.

Our efforts focused on optimizing parameters to achieve high-resolution printing at high speeds. Over 50 cavity configurations were investigated, with variations in size, depth, and spacing, to determine their impact on pattern transfer accuracy. The experiments utilized a dielectric ink, Poly(4-vinyl phenol) in propylene glycol monomethyl ether acetate, under varying viscosities and printing speeds.

B11. Tino Adrian Jucker

Clinical evaluation of an innovative air mattress for neonatal pressure ulcer prevention

Tino Adrian Jucker[1,2], Simon Annaheim[1], Martin Camenzind[1], Anna-Barbara Schlüer[3], Barbara Brotschi Aufdenblatten[4,5], René Michel Rossi[1,2]

[1] Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Biomimetic Membranes and Textiles, Lerchenfeldstrasse 5, St. Gallen, Switzerland

[2] ETH Zürich, Department of Health Sciences and Technology, Zürich, Switzerland

[3] Institut of Nursing, School of Health Sciences, Zurich University of Applied Sciences, Winterthur, Switzerland

[4] Department of Neonatology and Pediatric Intensive Care, University Children's Hospital Zurich, Zurich, Switzerland

[5] Children's Research center (CRC) of the University Children's Hospital Zurich, University of Zurich, Zurich, Switzerland

Neonates on intensive care units are vulnerable to pressure ulcers due to prolonged immobility, fragile skin, and limited capacity to communicate discomfort. Foam mattresses, the current standard of care, do not adequately mitigate the interface pressures that lead to pressure ulcers. Tailored solutions addressing these unique requirements are critically needed.

We aimed to assess the efficacy of a novel air mattress in reducing interface pressure and pressure ulcer risk compared to standard foam mattresses in the labratory and subsequently in a neonatal intensive care unit.

The air mattress, designed with three compartments for optimized pressure distribution, was evaluated through a laboratory study. Laboratory tests measured interface pressures under different body weights (1.3–3.3 kg) and air pressures (0.2–0.6 kPa) using a neonatal model. In the next development step, a Swissmedic and Swissethic accredited clinical trial was performed, including 23 neonates in a randomized crossover design, comparing air and foam mattresses over two 60-minute intervals. Interface pressures, stress (heart rate, SpO2, respiration rate), and subjective comfort were measured.

The air mattress significantly reduced interface pressure across all measured weights compared to foam mattresses ($p < 0.05$). For preterm models (1.3 kg), interface pressure was reduced significantly. Clinical findings also confirmed lower interface pressures in general, most prominent on the head area (35% reduction). The new mattress did not have any adverse impact on stress levels or comfort scores. There is a trend of a more rapid acclimatization of neonates to the novel air mattress, with stabilized vital signs observed within the first 30 minutes.

The innovative air mattress effectively reduces interface pressure and pressure ulcer risk in neonates, outperforming standard foam mattresses in the clinical trial. These findings highlight its potential as a tailored, preventive solution for neonates on the intensive care units, addressing critical gaps in current care.

B12. Matthias Klimpel

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

M. Klimpel[a,b]*, H. Zhang[a,b]*, K. Wieczerzak[c], R. Dubey[a,b], F. Okur[a,b], J. Michler[c], L.P.H. Jeurgens[d], D. Chernyshov[e], W. van Beek[e], K. V. Kravchyk[a,b], M. V. Kovalenko[a,b]

[a]Laboratory of Thin films and Photovoltaic, Empa Dübendorf,

[b]Laboratof of Inorganic Chemistry, ETH Zürich,

[c]Laboratory for Mechanics of Materials and Nanostructures, Empa Thun,

[d]Laboratory for Joining Technologies & Corrosion, Empa Dübendorf,

[e]Swiss-Norwegian Beamlines, European Synchrotron Radiation Facility, Grenoble

Ultrafast (UF) sintering emerges as a game-changing sintering methodology for fabricating $Li_7La_3Zr_2O_{12}$ (LLZO) solid-state electrolytes, representing a pivotal stride toward the advancement and prospective commercialization of Li-garnet solid-state batteries.[1, 2] Despite its widespread use in the fabrication of LLZO ceramics, the chemical composition of the UF-sintered LLZO surface remains largely unexplored. This study presents an in-depth analysis of the surface chemistry of UF-sintered LLZO. Our investigation uncovers a striking difference between the surface of UF-sintered and conventionally sintered LLZO, revealing predominant surface contamination by Li_2O in the case of UF processing. Comparative synchrotron X-ray diffraction data during UF and conventional sintering elucidate the origin of surface contamination. We propose a viable solution to this issue through an additional heat-treatment (HT) step at 900 °C after UF sintering. Furthermore, we present a comparative assessment of the electrochemical performance based on UF-sintered LLZO pellets, both with and without the post-HT step, underscoring the pivotal role of an uncontaminated LLZO surface.

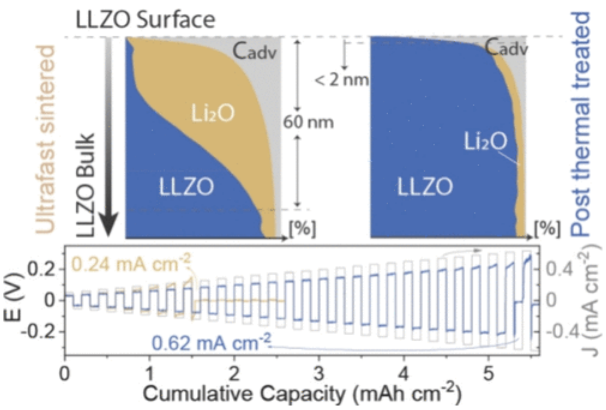


Fig. 1: *Comparison of the surface composition of garnet solid electrolyte pellets after ultra-fast sintering and after the post-thermal treatment. Less* Li_2O *leads to an improved electrochemical behavior.*

References

1. Kim, K. J.; et al. *Adv. Energy Mater.* **2021**, *11* (1), 2002689.

2. Wang, C.; et al. *Science* **2020**, *368* (6490), 521-526.

B13. Léo Lapeyre

Exploring Early-Stage Growth Dynamics of LiNbO3 by ALD on NMC 811 Cathodes: an In Situ QCM Analysis for Artificial SEI Applications

Léo Lapeyre[1]*, Amit Sharma[1], Arnold Müller[3], Laszlo Pethö[1], Patrice Raynaud[2], Johann Michler[1], Ivo Utke[1]

[1] *Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Mechanics of Materials and Nanostructures, Feuerwerkerstrasse 39, 3602 Thun, Switzerland*

[2] *Laboratoire Plasma et Conversion d'Energie (LAPLACE), Université de Toulouse, CNRS, INPT, UPS, 31062 Toulouse, France*

[3] *Laboratory of Ion Beam Physics, Department of Physics, ETH Zürich, 8093 Zurich, Switzerland*

Enhancing the performance and stability of high-energy lithium-ion batteries (LIBs) necessitates the deposition of effective cathode-electrolyte interphases (CEIs). Nickel-rich cathodes like NMC 811 suffer from interface degradation during cycling, requiring ultra-thin, conformal artificial CEIs to mitigate this issue. However, early-stage growth challenges in atomic layer deposition (ALD) hinder the development of ideal CEIs. This study addresses the challenges of substrate-induced nucleation delays, poor surface coverage, and chemical inhomogeneity during ALD growth of lithium niobium oxide (LNO) on NMC 811 cathodes limiting the protective capability of artificial CEIs. Using in situ quartz crystal microbalance (QCM), we investigated the initial growth dynamics of LNO films deposited from lithium tert-butoxide (LiOtBu) and niobium ethoxide (Nb(OEt)5) precursors. First, the impact of varying Li:Nb pulsing ratios on film stoichiometry and nucleation was evaluated. Island growth was observed during initial cycles, with film coalescence and full coverage occurring at a critical thickness (~15 nm). Poor surface coverage at lower cycle counts left the cathode vulnerable, while excessive thickness reduced lithium-ion conductivity. This thickness highlights a key trade-off: while thinner films offer higher lithium-ion conductivity, they fail to fully encapsulate and protect the NMC cathode surface. Our findings highlight the importance of selecting adapted ALD precursors to address substrate-induced growth challenges, ensuring chemically uniform and conformal coatings for effective CEI design. This work provides a powerful method for optimizing ALD processes for NMC811 and other battery materials, enabling superior electrochemical performance and longevity in next-generation lithium-ion batteries.

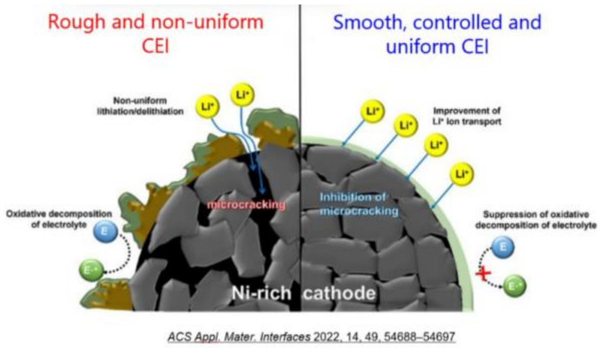


Figure 1: Schematic of CEI formation and interface degradation during cycling of Ni-rich cathodes vs. controlled artificial CEI deposited by ALD.

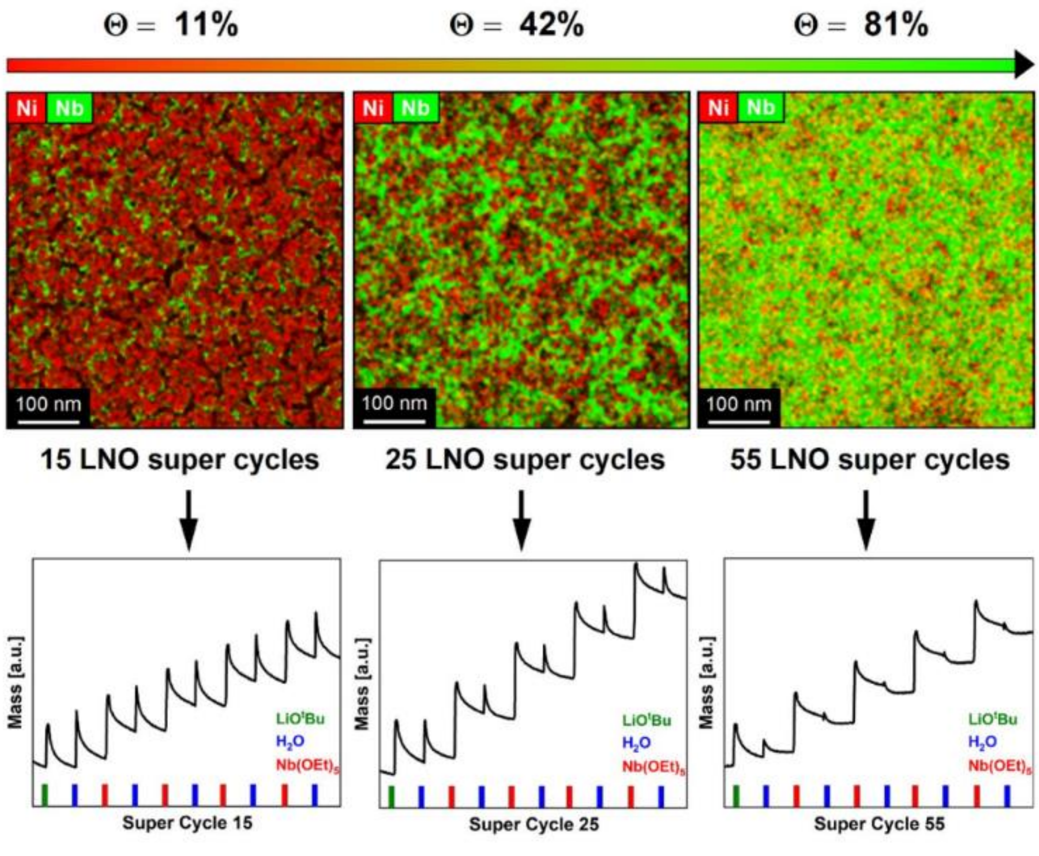


Figure 2: *TEM-EDX mapping of LNO coverage on NMC 811 at various stages of the deposition with related mass signal from QCM.*

B14. Jincheng Luo

Scalable Coating of Wide-Bandgap Perovskites on Flexible Substrates for Photovoltaic Application

Jincheng Luo[1*], Johnpaul Kurisinkal Pious[1], Severin Siegrist[1], Radha Krishnan Kothandaraman[1], Huagui Lai[1], Ioanna Vareli[1], Fan Fu[1]

[1]*Laboratory for Thin Films and Photovoltaics, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

INTRODUCTION: Metal halide perovskite solar cells (PSCs) are emerging as a promising next-generation photovoltaic technology, offering high power conversion efficiency (PCE), cost-effectiveness, and broad applicability. Wide-bandgap (WBG) perovskites are critical in constructing semi-transparent and multi-junction devices. Achieving uniform perovskite films on flexible substrates is crucial for developing flexible solar modules with a high power-to-weight ratio; however, it remains a significant challenge. Here, we utilized meniscus-based coating techniques for perovskite deposition, complemented by hole transport layer (HTL) modification to enhance the wettability of the perovskite ink. This approach enables the uniform deposition of WBG perovskites over large-area flexible substrates, ensuring consistent performance on cell scale. Furthermore, flexible WBG perovskite solar modules were fabricated, achieving an efficiency of over 10%. Finally, the coating process was successfully scaled up to 10 × 10 cm² substrates, demonstrating its potential for the fabrication of flexible all-perovskite multi-junction solar modules in the next step.

METHODS: Perovskite ink is coated onto PEN/ITO/NiO_X/self-assembled monolayer (SAM) stacks via blade-coating or slot-die coating, followed by drying with an air knife. Photoluminescence and UV-vis spectroscopy are employed to assess the quality and uniformity of perovskite films. For device fabrication, C_{60}, BCP and Cu are sequentially deposited through thermal evaporation. Device performance and its spatial homogeneity are evaluated using current-voltage measurements under simulated AM 1.5 G solar illumination with an irradiance of 100 mW cm^{-2}.

Fig. 1: *Photos of a WBG perovskite solar module (left) and a semi-transparent WBG perovskite film (right).*

RESULTS & DISCUSSION: NiO_X is inserted between SAM and ITO to regulate the SAM growth, thereby enhancing the wettability of perovskite ink on SAM. This approach enables the formation of uniform WBG perovskite films on flexible substrates using blade-coating. After screening various SAMs, the NiO_X/Me-4PACz bilayer was selected as the HTLs, resulting in efficient flexible solar cells and modules with champion PCEs of 16.7% and 10.3%, respectively. Furthermore, this strategy can also be applied to deposit perovskite films using slot-die coating, with scalability demonstrated on 10 × 10 cm² flexible substrates.

CONCLUSIONS: The NiO_X/Me-4PACz bilayer effectively promotes uniform WBG perovskite coating on flexible substrates, enabling efficient PSCs with excellent homogeneity. This strategy can also be applied with slot-die coating uniform large-area deposition, advancing flexible photovoltaic module technology.

ACKNOWLEDGEMENTS: This work received funding from the European Union's Horizon Europe research and innovation program under grant agreement no 101075605 as well as from the Swiss National Science Foundation (no.

200021_213073) and Swiss Federal Office of Energy (SI_502549-01).

B15. Philipp Meier

Safety and sustainability assessment of antiviral, antibacterial and antifungal nanocoatings applied on porous- and non-porous surfaces

Philipp Meier[1], Peter Neubauer[2], Peter Wick[1]*

[1] *Materials in Health Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, Switzerland*

[2] *Chair of Bioprocess Engineering, Institute for Biotechnology, TU Berlin, 13355 Berlin, Germany*

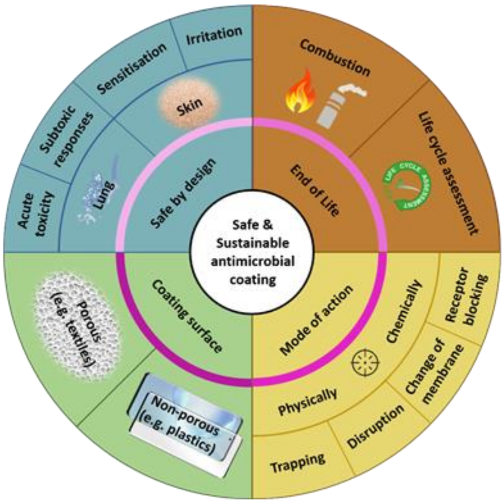


Fig. 1: *Simplified PhD project objectives.*

INTRODUCTION: While the global healthcare system is recovering from COVID-19 pandemic, new multi-drug resistant pathogens are emerging as the next threat. To tackle these challenges there is a need for safe and sustainable antimicrobial functionalized materials.

METHODS: Here we develop a procedure for the surface functionalization of textiles. A quaternary ammonium-based coating was applied homogeneously onto hospital curtains. Abrasion, durability testing, and aging resulted in little change on the performance of the treated textile[1].

RESULTS & DISCUSSION: Qualitative and quantitative antibacterial assays revealed an excellent antimicrobial activity with a CFU reduction of 98 - 100%. The treated curtain was aged 6 months prior to testing. Similarly, the antiviral activity showed >99% viral reduction with the functionalized curtain. The released chemical from the coating revealed no acute in vitro skin toxicity (IC_{50}: 95 µg mL^{-1}) and sensitization.

CONCLUSIONS: The BASF coating illustrated a high antibacterial and antiviral efficacy when applied onto a porous surface carrier such as textiles. The safety assessment revealed no skin irritation or sensitization potential in the applied concentration range. Further studies regarding the ‘end of life’ via incineration should be performed to assess the ecological impact of such novel metal-free antimicrobial coatings.

ACKNOWLEDGEMENTS: The authors would like to thank the 403 Materials in Health team. Additionally, we thank Jörg Gschwend and Stefan Gfeller from Empa for designing and construction of the customized Sheffield head filter membrane holder for the fibre analysis. The paper was conducted with funding from BASF - Schweiz.

REFERENCES:

1. P. Meier et al. *Environ. Int.* **2022**, *167*, 107364.

B16. Ceren Mitmit

Semi-transparent Wide-Bandgap ACIGS Solar Cells by Low Temperature Processes

Ceren Mitmit[1], Matthias Diethelm[1], Romain Carron[1]

[1] *Laboratory for Thin Films and Photovoltaics, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

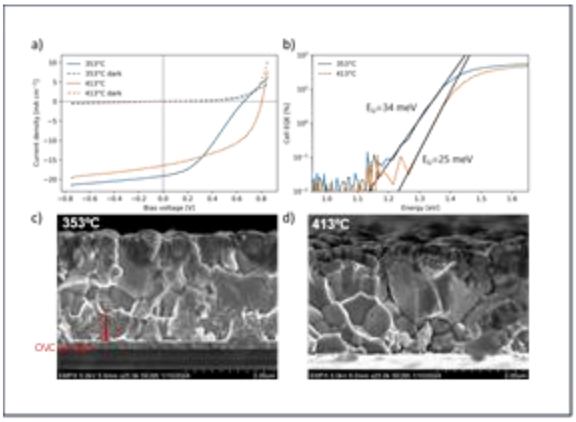


Fig. 1: *Effect of deposition temperature on devices.*

INTRODUCTION Tandem solar cells exceed the performance limit of single-junction devices, offering scalable, cost-effective solution for energy generation and power the world. Chalcogenide thin films are ideal for tandem devices due to their tunable bandgap, strong absorption coefficient, long-term stability, and flexibility.[1,2] This study explores the manufacturing limit for deposition temperature for wide-bandgap ACIGS and manipulation of the compositional gradients aiming at mitigating the non-radiative recombination losses at the back contact.

METHODS: Ag was thermally evaporated onto ITO-coated glass. CIGS absorbers were grown via 3-stage co-evaporation, followed by in-situ NaF and RbF PDTs. CdS was deposited via CBD, and devices were finalized with i-ZnO/AZO layers by sputtering and Ni-Al grids by e-beam evaporation.

RESULTS & DISCUSSION: We observed a so-called ordered vacancy compound (OVC) phase at the back of the absorber deposited at 353°C, due to slower Cu in-diffusion during co-evaporation. Increasing the temperature to 413°C enhances Cu diffusion, prevents the formation of the OVC phase, and improves material quality, yielding ~120 mV V_{OC} gains and higher FF. However, at 453°C, device performance degrades. Additionally, we demonstrate how to manipulate compositional gradients aiming to reduce non-radiative recombination at the back contact.

CONCLUSIONS: Optimizing deposition temperature improves absorber quality, prevents OVC phase, and enhances device performance. Compositional gradients in wide-bandgap ACIGS can mitigate recombination losses and improve bifacial performance, making them suitable for tandem applications.

ACKNOWLEDGEMENTS: *Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or CINEA. Neither the European Union nor the granting authority can be held responsible for them (Project 101075626 "SITA")*

REFERENCES:

(1) Larsson, F.; Nilsson, N. S.; Keller, J.; Frisk, C.; Kosyak, V.; Edoff, M.; Törndahl, T. Record 1.0 V Open-Circuit Voltage in Wide Band Gap Chalcopyrite Solar Cells. Prog. Photovolt. Res. Appl. 2017, 25 (9), 755–763. https://doi.org/10.1002/pip.2914.

(2) Keller, J.; Stolt, L.; Donzel-Gargand, O.; Kubart, T.; Edoff, M. Wide-Gap Chalcopyrite Solar Cells with Indium Oxide–Based Transparent Back Contacts. Sol. RRL 2022, 6 (8), 2200401. https://doi.org/10.1002/solr.202200401.

B17. Vittorio Montanelli

Microstructural Studies of Thin Film All-Solid-State Batteries by S/TEM

Vittorio Montanelli[1], Jędrzej Morzy[2], Yaroslav E. Romanyuk[2] and Marta D. Rossell[1]

[1] *Electron Microscopy Center, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Laboratory for Thin Films and Photovoltaics, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

INTRODUCTION: All-solid-state batteries (ASSBs) are considered a promising solution to the safety issues and energy density limitations of conventional Li-ion batteries (LIBs) containing liquid electrolytes. The employment of solid electrolytes with wider electrochemical windows allows the use of high-capacity Li-metal anodes and high-voltage cathode materials to achieve higher energy and power densities. However, undesirable physical and chemical interactions at solid electrolyte/electrode interfaces lead to significant differences between predicted and actual ASSB performances, hindering their large-scale commercialization. These interfacial issues occur at the nanoscale, making scanning transmission electron microscopy (S/TEM) a powerful tool to study them.

METHODS: A completely airless workflow is introduced for the sample preparation and analysis. TEM lamellas from the thin-film batteries are prepared by focused ion beam (FIB) on MEMS chips. The chips are then mounted on an air-free transfer TEM holder which allows electrical biasing. The micro-batteries are then investigated using S/TEM imaging, diffraction and spectroscopytechniques, i.e. EDX and EELS.

RESULTS & DISCUSSION: This work focuseson the effects of flash lamp annealing (FLA) during the preparation of thin-film ASSBs with NMC811 cathodes (Fig. 1). Compared to the non-annealed sample, the FLA-sample exhibits delamination between the cathode and the current collector, along with the presence of vertical cracks in the cathode. Diffraction experiments show that FLA-NMC811 generally has a higher crystallinity, which decreases near the interface with the solid electrolyte.

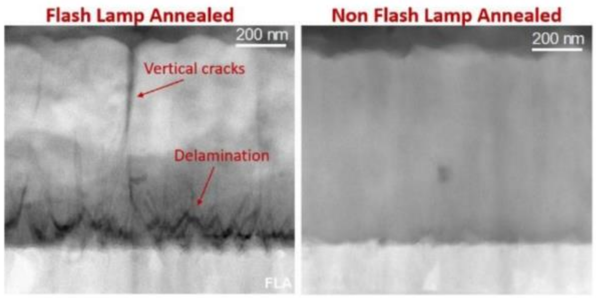


***Fig. 1:** HAADF images of FLA and non-FLA samples. From bottom to top: Ti current collector, NMC811 cathode, and LiPON solid electrolyte.*

CONCLUSIONS: The microstructure of NMC811 cathodes is investigated using various S/TEM techniques to reveal the effects of the FLA process on the crystallinity of the material. The established procedure for sample preparation and analysis will enable future studies on other battery types. Moreover, the experimental setup supports in-situ biasing experiments that can provide a deeper understanding of how, where and when degradation mechanisms and battery failure occur.

ACKNOWLEDGEMENTS: This work has been funded by the SNF under Project No. 200021_219706

B18. Saketh Ravuri

Nanographene based building blocks for tailoring magnetic phases

Saketh Ravuri[1], Chenxiao Zhao[1], Pascal Ruffieux[1], Roman Fasel[1]

[1] *Nanotech@surfaces 205, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

Motivation: Magnetism can be introduced in graphene nanoflakes or nanographenes, through sublattice imbalance, topological frustration, and electronic interactions. Leveraging the advantage of on-surface synthesis (OSS), we fabricate nanographenes with various geometries having different ground state magnetization, such as triangulene (S=1), olympicene (S=1/2), and Clar's goblet (S=1/2)[1][2]. These building blocks enable the realization of both ferromagnetic and antiferromagnetic spin chains, serving as ideal platforms for investigating exotic quasiparticles such as spinons and triplons, as well as distinct topological phases.

Problem Statement: Spin excitations in spin-½ antiferromagnetic Heisenberg chains have been studied under open-boundary conditions (OBC). However, excitation gaps vary depending on boundary conditions[2]. A systematic investigation comparing spin behavior across different chain lengths under periodic boundary conditions (PBC) is still lacking. Bridging this gap is crucial for advancing nanographene-based quantum simulators and spintronic applications.

Planned Approach: We fabricate 1D nanographene spin chains via on-surface synthesis on an Au(111) substrate, followed by polymerization and cyclization through annealing. Characterization is performed using Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) to probe spin excitations. To support experimental observations, we apply theoretical models, including Mean-Field Hubbard tight binding, Density Functional Theory (DFT), and Density Matrix Renormalization Group (DMRG). By systematically comparing OBC and PBC configurations, we aim to elucidate the role of boundary conditions in spin excitations and their impact on quantum properties. We can further extend OSS to study exotic quasiparticles and distinct topological phases in spin chains.

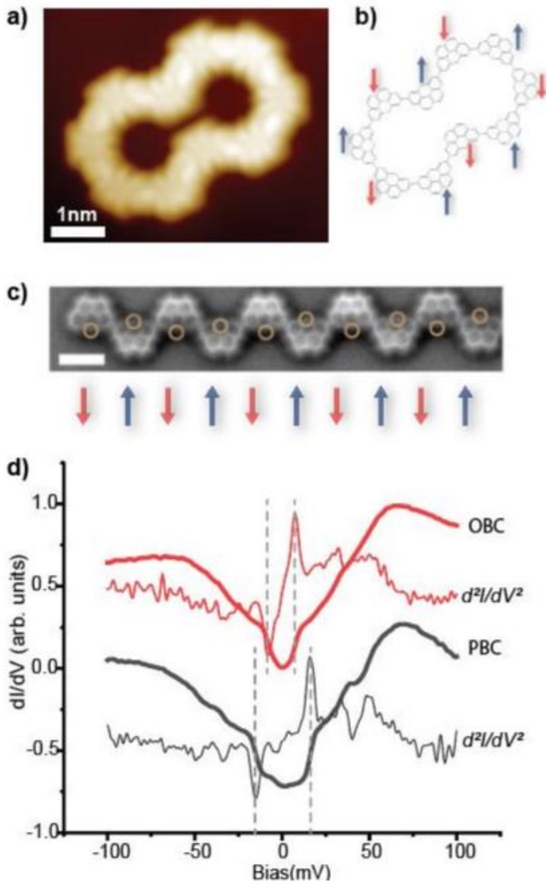


Fig. 1: *a, STM image of a 10-unit periodic-boundary ring (CO-functionalized tip). b, Chemical structure of (a). c, Atomic force microscopy image of a 10-unit open-boundary chain. d, STS spectra showing excitation gaps for PBC and OBC.*

References:

[1] Mishra, S. Catarina, G., Wu, F Ortiz, R et al. Nature, 598(7880), 287-292.https://doi.org/10.1038/s41586-021-03842-3
[2] Zhao, C. Yang, et al. arXiv:2408.10045

B19. Sina Ruhstaller

Prenatal origin of allergies: Can early-life environmental co-exposures to micro-/nanoplastics and allergens induce immune changes at the maternal-placental-fetal interface?

Sina Ruhstaller[1], Tina Bürki-Thurnherr[1]

[1] Nanomaterials in Health Lab, Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, Switzerland

INTRODUCTION: Microplastics have been found in every part of the human body and are thus global contaminants of great concern (low degradation rate, fragmentation & potential to take up pathogens) [1-6]. Little is known about how micro-/nanoplastics (MNPs) impacts the health of pregnant women and if these particles can be one of the environmental factors contributing to the increasing prevalence of allergies in newborns [5,7,8]. We are tackling the critical yet largely unexplored challenge of uncovering the health hazards posed by environmentally relevant MNPs during pregnancy.

METHODS: To achieve results predictive for human pregnancy, we employ different human-based placenta models (e.g. explant cultures or static and dynamic co-culture models) using 1. and 3. Trimester placenta tissue obtained from the local hospitals. Additionally, we generate real-life MNP materials through milling or abrasion of consumer plastic products and plastic litter collected by The Ocean Cleanup directly from the ocean surface.

RESULTS & DISCUSSION: A successful production of different MNP samples (polypropylene, high- and low-density polyethylene & Ocean Cleanup particles) could be achieved. Initial physical-chemical characterization indicate the presence of polydisperse samples in the nano- to micrometer size range.

CONCLUSIONS: We will now continue to investigate MNPs interaction with different allergens their effects on placental immune/endocrine functions and their potential prenatal priming of allergies in later life.

Illuminating our understanding of the potential health risks of MNPs during pregnancy is crucial for ensuring the sustainable production and use of plastics and safeguarding the health of pregnant women and unborn children.

ACKNOWLEDGEMENTS: We would like to thank The Ocean Cleanup for providing us with more realistic samples. Benno Wüst or the help with milling of plastics. As well as our other collaboration partners such as BRAVE analytics, Denise Mitrano, KSSG and Sails & Explore Association.

REFERENCES:

[1] Ragusa, A., et al., Plasticenta: First evidence of microplastics in human placenta. Environ Int, 2021. 146: p. 106274.

[2] Braun, T., et al., Detection of Microplastic in Human Placenta and Meconium in a Clinical Setting. Pharmaceutics, 2021. 13(7).

[3] Fournier, S.B., et al., Nanopolystyrene translocation and fetal deposition after acute lung exposure during late-stage preg-nancy. Part Fibre Toxicol, 2020. 17(1): p. 55.

[4] Mitrano, D.M., P. Wick, and B. Nowack, Placing nanoplastics in the context of global plastic pollution. Nat Nanotechnol, 2021. 16(5): p. 491-500.

[5] Bouwmeester, H., P.C.H. Hollman, and R.J.B. Peters, Potential Health Impact of Environmentally Released Micro- and Nanoplastics in the Human Food Production Chain: Experiences from Nanotoxicology. Environmental Science & Technology, 2015. 49(15): p. 8932-8947.

[6] Lehner, R., et al., Emergence of Nanoplastic in the Environment and Possible Impact on Human

Health. Environmental Science & Technology, 2019. 53(4): p. 1748-1765.

[7] Warner John, O., The foetal origins of allergy. Current Allergy & Clinical Immunology, 2017. 30(2): p. 62-68.

[8] Liu, S., et al., Eco-corona formation and associated ecotoxicological impacts of nanoplastics in the environment. Sci Total Environ, 2022. 836: p. 155703.

B20. Hauke Schlesier

Recycling fossil infrastructure for greener energy transitions

Hauke Schlesier[1], Gonzalo Guillén Gosálbez[2], Harald Desing[1]

[1] Empa - Swiss Federal Laboratories for Materials Science and Technology, Technology and Society Laboratory, Lerchenfeldstrasse 5, 9014 St. Gallen, Switzerland

[2] Sustainable Process Systems Engineering Lab, Institute for Chemical and Bioengineering (ICB), Department of Chemistry and Applied Biosciences, Eidgenössische Technische Hochschule (ETH) Zürich, Vladimir-PrelogWeg 1-5/10, 8093 Zürich, Switzerland

The urgency of the accelerating climate crisis mandates to defossilize energy supply. Building the renewable energy infrastructure necessary requires large amounts of materials, the primary production of which causes environmental damage and impacts on local communities. Secondary production of bulk metals can reduce environmental damage but is limited by the availability of scrap. Here we map material stocks contained in soon-to-be-obsolete fossil infrastructure and explore the poorly understood potential of recycling them using life cycle assessment and monetization of impacts. Steel is the largest stock of metals (~1 Gt), which matches demand for steel required in transition pathways. Recycling of steel alone would allow to save up more than 2 Gt CO_2, eq emissions and up to 12 trillion $US externality costs. The earlier recycling happens, the lower externality costs. Using recycled steel for wind turbines and photovoltaic mounting systems, can reduce climate impacts of by 24% and 26% respectively. Given the strong quantitative evidence of the advantages of recycling fossil infrastructure, policies should ensure that recycling happens as soon as they become obsolete.

B21. Katharina Sribike

A dynamic dECM-based hydrogel for in vitro tissue models

Katharina Sribike[1,2,3,4], Markus Rottmar[2], Marija Buljan[1,5], Katharina Maniura[2,4], Kongchang Wei[2,3]

[1] Laboratory for Particles-Biology Interactions,

[2] Laboratory for Biointerfaces,

[3] Laboratory for Biomimetic Membranes and Textiles, Empa, Swiss Federal Laboratories for Materials Science and Technology , Lerchenfeldstrasse 5, 9014 St. Gallen, Switzerland

[4] Department of Health Sciences and Technology, ETH Zurich, Zurich, Switzerland

[5] SIB, Swiss Institute of Bioinformatics, Lausanne, Switzerland

INTRODUCTION: 3D in vitro systems are becoming increasingly popular for their ability to mimic tissue structures and bridging the gap between simplistic 2D cell culture models and animal models[1]. Hydrogels are essential tools for 3D disease modeling and drug testing due to their tunable properties and ability mimic complex cell interactions[2]. Commonly used hydrogels include Matrigel, collagen, or alginate, which are limited in terms of me-chanical properties and xenogenicity[3]. Decellularized ECM (dECM) hydrogels replicate native ECM biochemistry of the tissue more accurately but often rely on cytotoxic crosslinkers such as glutaraldehyde, which restricts their applicability. Dynamic hydrogels, crosslinked with non-covalent interactions, support degradation independent cell activities, including 3D cell spreading and migration[4-5]. However, dynamic crosslinking strategies for dECM-based hydrogels are still lacking.

METHODS: Our experiments employed porcine skin as an ECM source, being decellularized using freeze-thaw cycles and subsequent Tween and SDS treatment. The resultant dECM was cryogenically ground, solubilized, and mixed with Ac-β-CD to form a dynamic host-guest complex. UV-initiated polymerization of acrylate groups in the precursor solution resulted in hydrogel formation.

RESULTS: We show that Ac-β-CD-clustering is able to crosslink dECM into host-guest hydrogels, achieving tunable mechanical properties. We demonstrate the modularity and tunability of the hydrogel properties in regard to its composition and Ac-β-CD concentration, achieving increasing stiffness with increasing Ac-β-CD concentration. The dynamic nature of the formed host-guest hydrogel becomes clear when comparing the negligible damping factor of a static equivalent hydrogel (GelMa) to the increased damping factor values in the host-guest hydrogels, indicating a viscoelastic solid-like behavior with dominant elastic properties but non-negligible viscous dissipation.

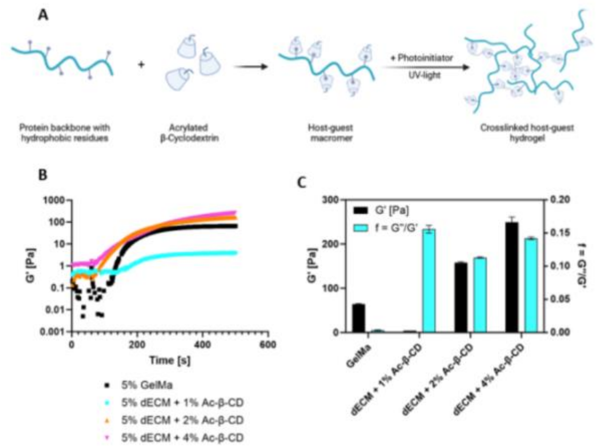


Figure 1: *(A) Ac-β-CD-assisted dECM crosslinking mechanism. (B) UV-Curing of gelatin- and dECMbased dynamic and static hydrogels in the presence of I2959 as photoinitiator (C) Rheological properties of static and dynamic hydrogels with varying ratios of Ac-β-CD.*

DISCUSSION & CONCLUSIONS: Our findings support the notion that host-guest-crosslinked dECM hydrogels present a viable platform for creating dynamic, physiologically relevant 3D tissue models.

REFERENCES:

[1]Chaicharoenaudomrung, et al. (2019). Three-dimensional cell culture systems as an in vitro platform for cancer and stem cell modeling. World journal of stem cells,

[2]Kyriakopoulou, et al. (2023) Recreating the extracellular matrix: novel 3D cell culture platforms in cancer research. The FEBS Journal.,

[3]Vitale, et al. (2022) Tumor Microenvironment and Hydrogel-Based 3D Cancer Models for In Vitro Testing Immunotherapies. Cancers.,

[4]Feng, et al. (2019) Dynamic and Cell-Infiltratable Hydrogels as Injectable Carrier of Thera-peutic Cells and Drugs for Treating Challenging Bone Defects. ACS Central Science;

[5]Feng, et al. (2016) Mechanically resilient, injectable, and bioadhesive supramolecular gelatin hydrogels crosslinked by weak host-guest interactions assist cell infiltration and in situ tissue regeneration. Biomaterials.

B22. Dan Stefanita

Improving local antibiotic therapy through the study of interactions and release mechanisms between $CaSO_4$ carriers and antibiotics

Dan Stefanita[1,2], Sabrina L. J. Thomä[1], Damien Terebenec[1], Peter Wahl[3,4], Antonia Neels[1,2]

[1] *Center for X-ray Analytics, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland*

[2] *Department of Chemistry, University of Fribourg, Fribourg, Switzerland*

[3] *Faculty of Medicine, University of Bern, Bern, Switzerland*

[4] *Division of Orthopaedics and Traumatology, Cantonal Hospital Winterthur, Winterthur, Switzerland.*

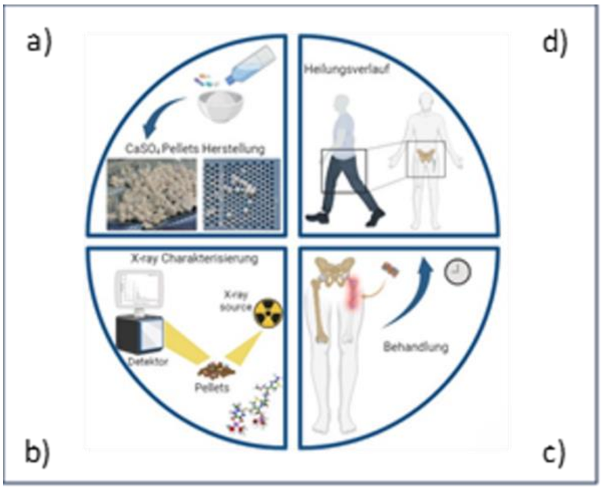


Fig. 1: *Summary of samples preparation (a) and analytical characterisation (b) vs. treatment (c) and healing process (d).*

INTRODUCTION: The treatment of infections in orthopaedic and trauma surgery remains a major challenge in modern medicine.[1] Local antibiotic therapy plays a significant role in the overall treatment of bone and joint infections.[2,3] This study investigates the structural and morphological features of local drug delivery systems using calcium sulfate ($CaSO_4$) as a carrier material for antibiotics like vancomycin[2] and ceftriaxo-ne[2,3].

METHODS: The research applies a multi-faceted approach, utilizing X-ray diffraction, spectroscopy, and FTIR analysis to characterize drug-carrier interactions at the molecular level. Thermogravimetric analysis reveals the hydration state and thermal stability of the Ca-Ceftriaxone complex, while pH analysis provides insights into the chemical nature of these compounds in solution.

RESULTS & DISCUSSION: Pair Distribution Function (PDF) analysis of nano-crystalline Ca-Ceftriaxone shows similar short-range ordering to Na-Ceftriaxone heptahemi-hydrate in water, with altered intensity ratios and an additional Ca-O distance correlation. The absence of sulfate anions is confirmed by the missing characteristic S-O distance.

CONCLUSIONS: This comprehensive study of antibiotic-$CaSO_4$ interactions provides crucial insights into the binding mechanisms within the crystalline structure. While future work may explore drug delivery aspects, the current focus on powder diffraction and crystal structure analysis lays the basis for understanding how the $CaSO_4$ matrix influences antibiotic properties. These findings contribute to the development of improved local antibiotic therapies,[2,3] potentially enhancing infection management and patient outcomes in orthopaedic and trauma surgery.[1]

REFERENCES:

1. Gramlich, Y., T. Johnson, M. Kemmerer, G. Walter, R. Hoffmann and A. Klug (2020), Knee Surg. Sports Traumatol. Arthrosc. 28(9): 2823-2834.

2. Wahl, P., K. Rönn, M. Bohner, L. A. Decosterd, C. Meier, M. Schläppi, S. Festa, E. Gautier, (2018), J. Bone Joint Infect. 3(4), 212-221.

B23. Xue Sun

Translating Planetary Boundaries into Material-Level Life Cycle Assessments

Xue Sun[1], Stephan Pfister[2], Roland Hischier[1]

[1] *Technology & Society Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, St.Gallen, Switzerland*

[2] *Chair of Ecological Systems Design, ETH Zürich, Zürich, Switzerland*

INTRODUCTION: As global environmental degradation accelerates, the Planetary Boundary (PB) framework provides a critical lens to evaluate social activities against ecological and geophysical flow limits. However, translating this global framework then into actionable methodologies that allocate limits at material- and material's use-pattern (product-) level remains challenging, particularly during the development of new materials from early stages.

METHODS: This contribution presents the so-called Material Boundary Availability (MBA) method, adapted from the Ecological Resource Availability (ERA) method by Desing et al. (2020). Unlike ERA, MBA incorporates also the use phase of materials, extending assessments to the product-level in order to provide a more comprehensive perspective. It allocates portions of PBs (e.g., CO_2 emissions) to individual materials and their use-patterns (products), considering production and consumption shares alongside environmental impacts. These allocations are iteratively scaled until a PB is exceeded at a given probability, defining maximum sustainable volumes.

MBA replaces ERA's historical *Grandfathering* principle with a *Sufficiency-based allocation* principle rooted in fulfilling basic needs and promoting a fair transition to sustainability. The method identifies materials and products most at risk of exceeding PBs. Visualizations, such as heatmaps are used to understand key factors, support regulatory decision-making, and guide informed industry practices.

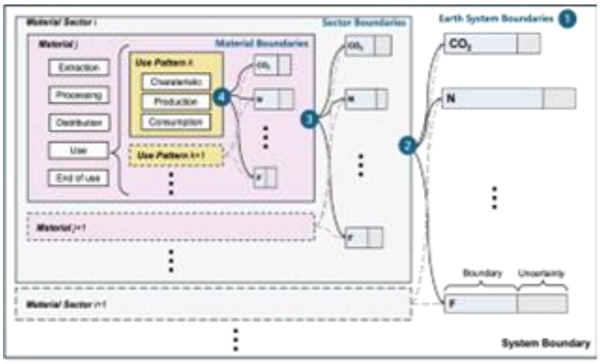


Fig. 1: *Schematic Representation of the Material Boundary Availability (MBA) Method. (1) selection of Earth system boundaries; (2) allocation of safe operating space (SOS) across material consumption sectors; (3) allocation of SOS for individual materials; and (4) allocation of SOS for specific material use-patterns. Steps 2-4 involve iterative calculations across subsystems to achieve detailed, material-level allocations.*

CONCLUSIONS: The MBA method identifies materials and products with significant PB burdens, guiding policy and industry toward impactful sustainability interventions. For instance, developing material-level sustainability standards in future work will offer valuable insights to support global sustainability guidelines. Challenges remain on how to model sustainability for materials, products and sufficiency scenarios more comprehensively.

ACKNOWLEDGEMENTS: This study was supported by EU Horizon Project CHIASMA.

REFERENCES:

Desing, H., Braun, G., & Hischier, R. (2020). https://doi.org/10.1017/sus.2020.26

B24. Nikolaos Tagaras

A nanomedicine challenge under the radar: a case study of Mn@PCN224 nanozyme biotransformation

Nikolaos Tagaras[1], Haihan Song[2], Vera M. Kissling[1], Alexander Gogos[1], Giacomo Reina[1], Weijun Tong[2], Tina Buerki-Thurnherr[1]*

[1] *Nanomaterials in Health Laboratory, Swiss Federal Laboratories for Materials Science and Technology (Empa), St. Gallen 9014, Switzerland*

[2] *MOE Key Laboratory of Macromolecular Synthesis and Functionalization, Department of Polymer Science and Engineering, Zhejiang University, Hangzhou 310058, China*

INTRODUCTION: Nanomedicine, a groundbreaking field, offers promising solutions to unresolved health challenges. While efficacy and toxicity are at the forefront of the evaluation of novel nanomedicines, their biostability upon entering a biological system is often overlooked. Understanding their mechanisms and fate is vital for the prediction and improvement of efficacy, biosafety and ultimately their translation into clinics. In this context, our project focuses on single-atom nanozymes (nanoparticles with enzyme-mimicking properties, that bear similarities with the active centre of natural enzymes, thus improving substrate affinity and catalytic activity) and their biotransformation fate, enzymatic activity and biosafety upon exposure to a complex biological system.

METHODS: The highly stable metal-organic framework (MOF) PCN224, composed of Zr6clusters and porphyrin (TCPP), was doped with Mn-atoms, assembling Mn-TCPP complexes (Mn@PCN224), which mimic the active centre of natural superoxide dismutase (SOD) enzymes. We explored biotransformation with a variety of characterization techniques and assessed the Mn@PCN224 toxicity (viability, hormone production, barrier integrity and oxidative stress) in an advanced human placenta in vitro model.

RESULTS & DISCUSSION: Mn@PCN224 experienced considerable structural and compositional degradation. Specifically, ICP-OES results demonstrated a dramatic Mn release (~90%) after 6h incubation in a placentarelevant biological medium. Moreover, UV-Vis and Raman spectroscopy revealed that Mn is released bound to TCPP. Despite the disintegration, the released Mn-TCPP maintained enzymatic activity, demonstrating the robust Mn-TCPP complex. Mn@PCN224 were internalized by cells without apparent cytotoxicity.

CONCLUSIONS: This study provides evidence that Mn@PCN224 undergo significant biological medium-induced disintegration, emphasizing the importance of a biostability assessment to control the biodegradation of nanozymes for biomedical applications.

ACKNOWLEDGEMENTS: This research received funding from the Swiss National Science Foundation (grant no. 206059) and from the National Natural Science Foundation of China (grant no. 22161132027).

B25. Elisabeth Tobler

Optimizing fresh fruit Supply Chains with Digital Twins

Elisabeth Tobler[1,2], Thijs Defraeye[1]*

[1] *Laboratory for Biomimetic Membranes and Textiles, Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, Switzerland*

[2] *Wageningen University and Research, Food Quality and Design, Department of Agrotechnology and Food Sciences, Wageningen, The Netherlands*

INTRODUCTION: Refrigerated transport in trailers is one of the key unit operations in fresh fruit supply chains. Their design and operation should ensure uniform airflow, temperature, and humidity within the cargo to preserve the quality of such perishable products [1], [2]. To safeguard supply chains, in-transit monitoring is a common strategy. In commercial supply chains, the typical practice is to place only one temperature sensor in each transport, usually on top of the pallet closest to the door-end side of the trailer. However, relying on a single temperature sensor is insufficient to provide a comprehensive view of the hygrothermal conditions throughout the entire cargo, which is crucial for preventing localized high-temperature zones.

METHODS & RESULTS: Taking a leap forward, we develop physics-based 3D models of refrigerated trailers loaded with fresh fruit and integrate gathered sensor data into them, a concept commonly referred to as digital twins. By simulating airflow and temperature dynamics within a trailer, these models provide unique and detailed insights into airflow patterns, and forecast fruit temperatures and quality at every location within the cargo and at every timepoint during transportation [3]. Comparing simulations with experimental results reveals a relative error of 1 to 20%, depending on the location inside the trailer.

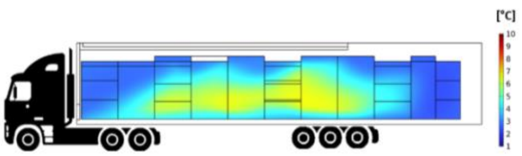


***Fig. 1:** 2D Contour plot illustrating a possible temperature distribution during refrigerated transport of fresh fruit.*

DISCUSSION & CONCLUSIONS: Digital Twins in fresh fruit supply chains enable stakeholders to quickly detect and address potential issues like poor air circulation or uneven cooling. By offering predictive insights, a digital twin helps to prevent potential problems before they escalate, ensuring that the perishable products arrive at their destination in optimal condition.

ACKNOWLEDGEMENTS: This work was financially supported by Sensitech, Coop Genossenschaft and Driscoll's, and subsidized by the Dutch Ministry of Economic Affairs and Climate Policy (EZK) through TKI Dinalog and the Topsector Logistics.

REFERENCES:

[1] J. Moureh, N. Menia, and D. Flick, "Numerical and experimental study of airflow in a typical refrigerated truck configuration loaded with pallets," *Comput Electron Agric*, vol. 34, no. 1–3, pp. 25–42, May 2002, doi: 10.1016/S0168-1699(01)00178-8.

[2] T. Yildiz, "CFD Characteristics of Refrigerated Trailers and Improvement of Airflow for Preserving Perishable Foods," *Logistics*, vol. 3, no. 2, p. 11, 2019, doi: 10.3390/logistics3020011.

[3] T. Defraeye, C. Verreydt, J. Gonthier, L. Lukasse, P. Cronjé, and T. M. Berry, "Building a physics-based virtual refrigerated container filled with fruit in ventilated packaging," *MethodsX*, vol. 13, no. September, p. 102984, 2024, doi: 10.1016/j.mex.2024.102984.

B26. Ziting Wang

Silicon carbide nanowires affect respiratory epithelial cell-mediated innate immune defense by impairing mucociliary functions

Ziting Wang[1], Jimmy Vernaz[2], Nikolaos Tagaras[1], Bernadett Boda[2], Tina Buerki-Thurnherr[1], Giacomo Reina[1], Vera M. Kissling[1], Samuel Constant[2], Govind Gupta[1], Peter Wick[1]

[1] *Laboratory for Particles-Biology Interactions, Swiss Federal Laboratories for Materials Science and Technology (Empa), CH-9014 St. Gallen, Switzerland*

[2] *Epithelix Sàrl, CH-1228 Geneva, Switzerland*

INTRODUCTION: Advanced materials (AdMs), such as silicon carbide nanowires (SiC NWs), exhibit unique properties but their safety for human health remains underexplored. This study assessed the respiratory toxicity and intracellular interactions of SiC using 3D bronchial epithelial cultures (HBE, MucilAir™) and compared them with reference materials like DQ12, SiO2, graphene, and MWCNTs.

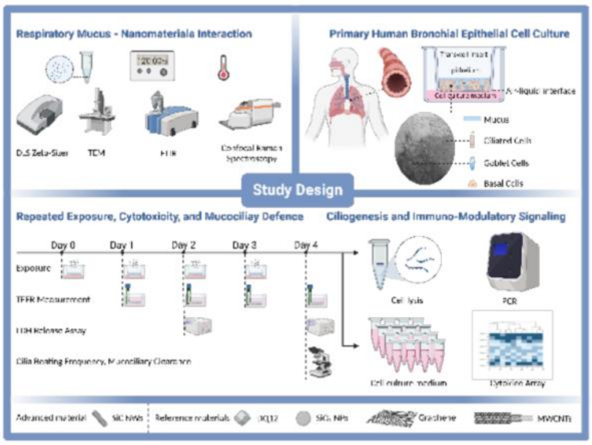


Figure 1: *Study design.*

METHODS: Physicochemical properties were characterized using zeta-sizer, TEM, and confocal-Raman microscopy. Biotransformation in the upper airway was studied by changes in surface charge, morphology, and functional groups after exposure to bronchial mucus. HBE cultures were exposed to materials for 4 days, with cell viability, integrity, and molecular responses assessed

RESULTS & DISCUSSION: The results from this study provide new insights on biotransformation and differential sub-toxic effects of silica and carbon-based NPs as well as AdMs on upper airway lung cultures. In addition, they highlight ciliary functions as a sensitive mechanism for particle-induced adverse effects.

CONCLUSIONS: SiC NWs don't induce acute cytotoxicity in the upper airway, but may have long-term effects.

ACKNOWLEDGEMENTS: Funding for this research was received from the EU Macramé project (Grant agreement number –101092686).

REFERENCES:

[1] Kennedy, et al. 2019. Risk Analysis, 39(8), pp.1783-1795

B27. Erfu Wu

A CMOS-Compatible Fabrication Approach for High-performance Perovskite Photodetector Arrays

Erfu Wu1, Sergey Tsarev2, Daria Proniakova2, Xuqi Liu2, Dominik Bachmann1, Sergii Yakunin2, Maksym V. Kovalenko2*, Ivan Shorubalko1*

1 Transport at Nanoscale Interfaces, Empa, Swiss Federal Laboratories for Materials Science and Technology, Dübendorf, Switzerland

2 Kovalenko Lab, ETH Zürich, Department of Chemistry and Applied Biosciences, Institute of Inorganic Chemistry, Switzerland

INTRODUCTION: Lead halide perovskites (LHPs) have attracted significant attention for their exceptional optoelectronic properties, positioning them as prime candidates for next-generation photodetectors (PDs). However, integrating these materials into device architectures with CMOS-compatible technologies in a simple manner remains a critical challenge.[1]

METHODS: This study introduces a universal method leveraging standard lithographic patterning to fabricate high-performance LHP PDs for red (R), green (G) and blue (B) color detection separately. Through optimization of the device stack and etching conditions, perovskite PDs are pixelated using a one-step lithography and pulsed argon (Ar) milling process.

RESULTS & DISCUSSION: The resulting devices exhibit typical perovskite PD responsivity (0.3 A W^{-1}), low dark current density (less than 10^{-6} mA cm^{-2}), high detectivity (over 10^{13} Jones) and short fall time (sub-20 ns without bias).

CONCLUSIONS: This approach not only enhances device performance but also paves the way for scalable production of perovskite-based optoelectronic devices. The versatility and effectiveness of this method highlight its potential for broad applicability in CMOS-compatible perovskite-based image sensor technology.

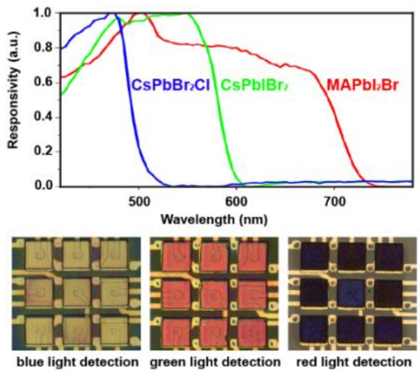


Fig. 1: *Top: Spectral responsivity of patterned perovskite PDs for red, green and blue light detection respectively. Bottom: Optical microscope images of patterned perovskite PDs. Pixel period is 25µm.*

ACKNOWLEDGEMENTS: The work was financially supported by ETH Zürich through the ETH+ Project SynMatLab: Laboratory for Multiscale Materials Synthesis.

REFERENCE:

1. L. Liang, T. Ma, Z. Chen, J. Wang, J. Hu, Y. Ji, W. Shen, J. Chen, Advanced Materials Technologies 2023, 8, 2200419.

B28. Yiwen Zhang

Using a Dynamic Probabilistic Material Flow Analysis Approach to Capture Japanese Plastic Flows

Yiwen Zhang[1], Zhanyun Wang[1], Masahiro Oguchi[2], Haruhisa Yamamoto[2], Bernd Nowack[1*]

[1] *Technology and Society Laboratory, Empa, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, Switzerland*

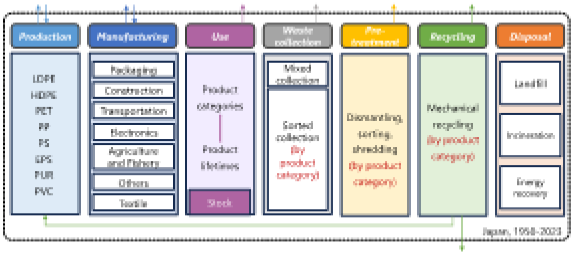
[2] *Material Cycles Division, National Institute for Environmental Studies, Japan*

INTRODUCTION: With stricter landfill regulations and increased demand for material efficiency, the Japanese plastic industry is now transitioning to a circular economy, aiming to reduce fossil-based plastic consumption and waste generation by applying various R-strategies. To achieve this, the first step is to understand the current plastic flows, with a particular focus on the waste management system. However, existing studies are not sufficient to provide such in-depth insights into the waste management of specific product categories, and a comprehensive investigation of all relevant industrial sectors and applications is lacking.

METHODS: In this study, we model the domestic plastic flows in Japan from 1950 to 2023, using a bottom-up Dynamic Probabilistic Material Flow Analysis (DPMFA) approach. Plastic stocks in use and waste streams are estimated according to historical activity data and corresponding product lifetimes. The model is solved 10,000 times using a Monte-Carlo method to present the variance of the model results.

RESULTS & DISCUSSION:

The model results present the detailed flows of plastics in the current waste management system and thus provide guidance for future research and action to enhance plastic circularity while ensuring the quality of secondary materials in Japan and other parts of the world.



B29. Zeyu Zhou

Effect of aluminium on the hydration and strength of MgO-nesquehonite binders

Zeyu Zhou[1,2]*, Ellina Bernard[1], Daniel Rentsch[1], Barbara Lothenbach[1,2]

[1] *Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Concrete and Asphalt, 8600 Dübendorf, Switzerland.*

[2] *University of Bern, Institute of Geological Sciences, Mineralogy Group, 3012 Bern, Switzerland.*

[3] *Empa, Swiss Federal Laboratories for Materials Science and Technology, Laboratory for Functional Polymers, 8600 Dübendorf, Switzerland.*

INTRODUCTION: Magnesium carbonate cements have shown significant potential as eco-friendly alternatives to Portland cement [1–3]. In particular, MgO/hydrated-magnesium-carbonate blends are more promising for ready-mix concrete due to the formation of hydrous carbonate-containing brucite (HCB) [4], resulting in a fast-strength development mechanism. Despite the promising results, the effect of different minor elements present in industrial raw materials or of supplementary cementitious materials (SCMs) on this binder has not yet been investigated systemically. Therefore, this study explores the impact of aluminum on Mg-silicate-carbonate binders by using metakaolin as a source of aluminate.

METHODS: Hydration study was carried out on paste samples. A high Mg/Si and Mg/Al ratio of 8 was used to in the cement paste production, to ensure enough Mg in the paste for hydration. X-ray diffraction (XRD), Fourier-transform infrared (FTIR) spectroscopy, thermogravimetric analysis (TGA) are used to characterize hydration products in the binders at different hydration period (1, 2, 7, 28 and 91 days). Compressive strength results was obtained from mortar specimen, produced and tested based on EN-196-3.

RESULTS & DISCUSSION: The X-ray diffraction (XRD) pattern confirms the existence of a hydrotalcite-like phase, $Mg_{2x}AlCO_3(OH)_{4+4x}\cdot(2+x)H_2O$, along with HCB and M-(A)-S-H during the formation. The formation of hydrotalcite-like phase allows more CO_2 sequestration and enhances strength. The CO_2 quantification via TGA analysis shows the binder can sequestrate up to 18 g of CO_2 per 100 g of dry cement. The tests on mortar prisms (water-to-binder ratio of 0.65) show 25 MPa at 2 days and above 35 MPa after 7 days.

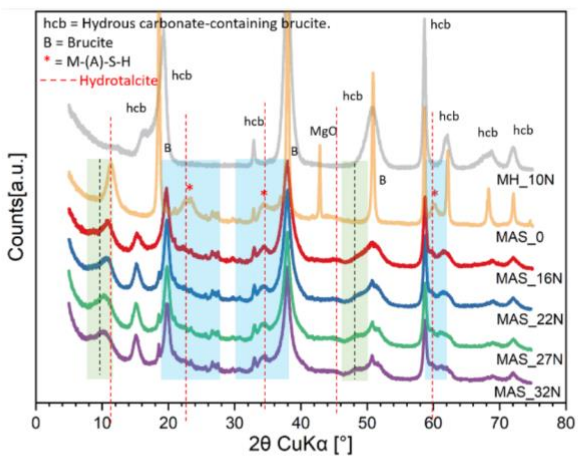


Fig. 1: *X-ray diffraction patterns of 91 days pastes of MH_10N, AMS_0, AMS_16, 22, 27, and 32N mixes.*

CONCLUSIONS: This study investigated the potential of incorporating metakaolin into Mg-carbonate binders, leading to the formation of hydrotalcite-like phases that enhance strength development and CO_2 sequestration. The binder demonstrated rapid strength gain, reaching over 35 MPa after 7 days, and achieved significant carbonation, sequestering up to 18 g of CO_2 per 100 g of dry cement. These findings demonstrate the potential of aluminium-rich supplementary materials to optimize magnesium-based cements, providing a sustainable alternative to conventional binders for eco-friendly construction.

ACKNOWLEDGEMENTS: The authors would like to express their thanks to Paula Monserrat Torres, Jan Schmitt, and Frank Winnefeld for their support and insightful discussion on MgO-nesquehonite binder systems. The financial support of the Swiss National Science Foundation (SNSF) under the SNSF Advanced 693 grant no. TMAG-2_209222 is sincerely acknowledged.

REFERENCES:

1. Bernard, E.; Nguyen, H.; Kawashima, S.; Lothenbach, B.; Manzano, H.; Provis, J.; Scott, A.; Unluer, C.; Winnefeld, F.; Kinnunen, P. MgO-Based Cements –Current Status and Opportunities. RILEM Technical Letters 2023, 8, 65–78, doi:10.21809/rilemtechlett.2023.177.
2. Abdel-Gawwad, H.A.; Hassan, H.S.; Vásquez-García, S.R.; Israde-Alcántara, I.; Ding, Y.-C.; Martinez-Cinco, M.A.; Abd El-Aleem, S.; Khater, H.M.; Tawfik, T.A.; El-Kattan, I.M. Towards a Clean Environment: The Potential Application of Eco-Friendly Magnesia-Silicate Cement in CO2 Sequestration. Journal of Cleaner Production 2020, 252, 119875, doi:10.1016/j.jclepro.2019.119875.
3. Lothenbach, B.; Bernard, E.; German, A.; Winnefeld, F. MgO-Based Binders. ce/papers 2023, 6, 342–356, doi:10.1002/cepa.2774.
4. German, A.; Winnefeld, F.; Lura, P.; Rentsch, D.; Lothenbach, B. Hydrous Carbonate-Containing Brucite (HCB) in MgO/Hydromagnesite Blends. Cement and Concrete Research 2023, 173, 107304, doi:10.1016/j.cemconres.2023.107304.

Sponsors of the event

Gold

BASF We create chemistry

Metrohm

venturelab

VENTURE KICK

Silver

ABB

CHEMLYS Creative chromatography

COMSOL

glatec | Empa eawag

Bronze

CARL ROTH

GMP PHOTONICS & MICROTECHNOLOGY

Quantum Design EUROPE