ETH zürich

MaP | Competence Center for Materials and Processes

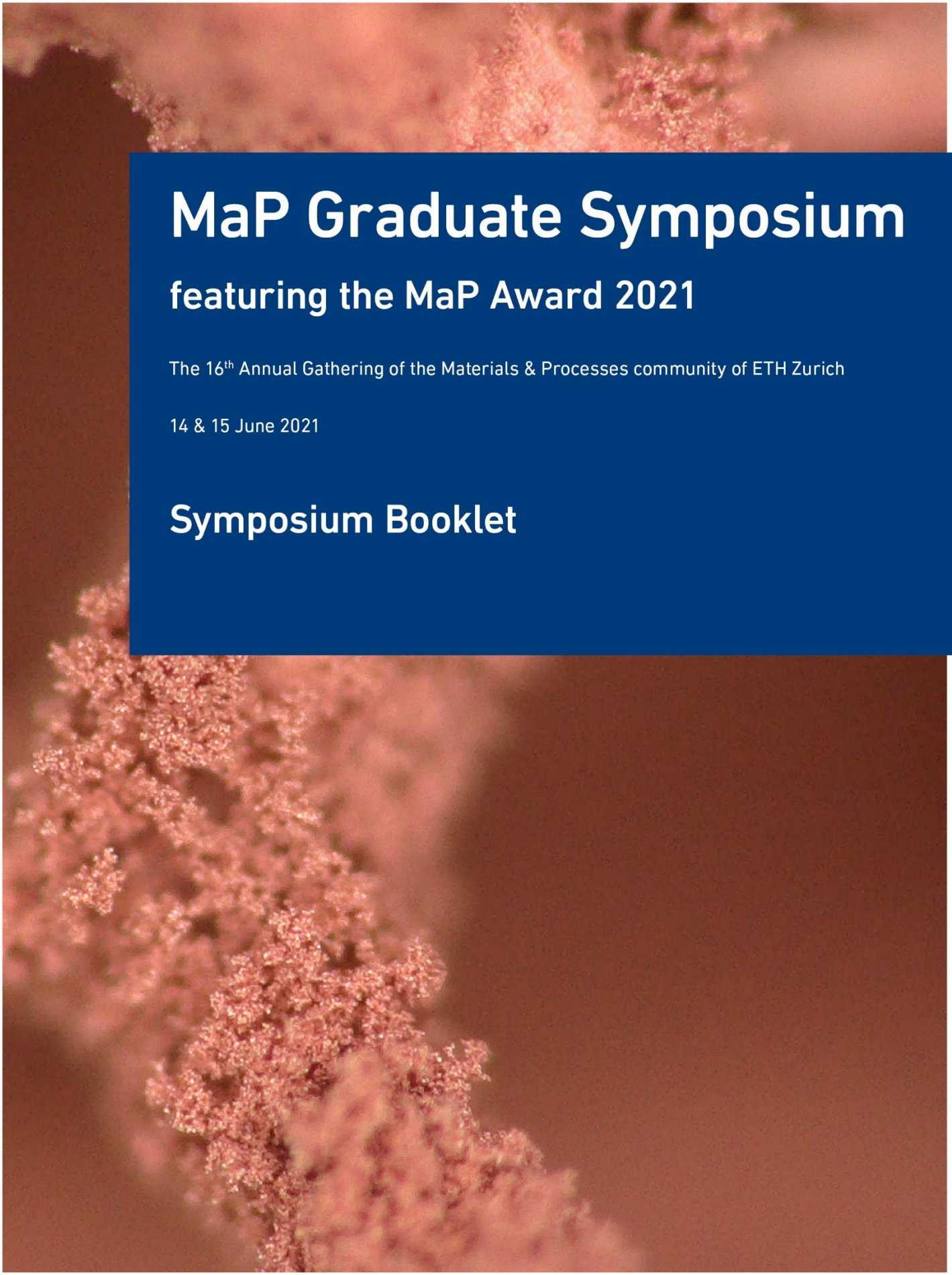
MaP Graduate Symposium

featuring the MaP Award 2021

The 16th Annual Gathering of the Materials & Processes community of ETH Zurich

14 & 15 June 2021

Symposium Booklet



Copper Cloud - Coating of a polymeric structure with copper nanoparticles // 2nd place picture of MaP Image Contest 2020 by Murielle Schreck (ETH Zürich)

Many thanks to our industry partners!

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Support

For assistance **before and after the symposium**, please reach out to the MaP office at map@mat.ethz.ch or +41 44 633 37 53.

During the symposium, helpdesks in ZOOM and on Gather.town will provide assistance.

Program

Monday 14 June 2021

13.00	**Opening**
Session 1: co-chaired by **Daniel Ahmed** (*D-MAVT*) & **Pernilla Andersson** (*Sensirion*)	
13.15	**Murielle Schreck,** *Multifunctional Materials, D-MATL* How 3D Printed Polymeric Scaffolds Influence Geometry, Mechanical Stability and Photocatalytic Performance of Nanoparticle-Based Aerogels
	Florin N. Isenrich, *Microfluidics & Nanoscale Science, D-CHAB* Towards a Golgi on a Chip
	Peter Benedek, *Materials & Device Engineering, D-ITET* Controlling Li Lithium Ion Battery (de)Intercalation Dynamics Through Interface Design
	Philipp Fisch, *Tissue Engineering & Biofabrication, D-HEST* Formation of Elastic Cartilage in Bioprinted Auricles
	Ariane Stucki, *Bioanalytics Group, D-BSSE* Two-Level Compartmentalization for Triggered Reagent Delivery in Double Emulsions
	MaP Mastermind Quiz #1
14.25	*Break*
MaP Award 2021	
14.35	**Dr. Chiao-Peng Hsu,** *Soft Materials & Interfaces, D-MATL* Tribological Insights into Shear Thickening Suspensions
	Dr. Philippe Grönquist, *Wood Materials Science, D-BAUG* Smart Manufacturing of Curved Mass Timber Components by Self-Shaping
	Dr. Tino Matter, *Nanoparticle Systems Engineering, D-MAVT* Uniting Bioactivities in Hybrid Nanosystems for Wound Healing
15.45	**Poster Session**
16.45	*Break*
16.55	**Award Ceremony** Industry Poster Awards, MaP Award
17.10	**Closing & Social Gathering**
17.30	End of Symposium Day 1

program element on Gather.town (for additional instructions, please see page 6)

Tuesday 15 June 2021

13.00	**Opening**
Session 2: co-chaired by **Eleni Chatzi** (*D-BAUG*) & **Adelina Braun** (*Merck*)	
13.05	**Johannes Weichart,** *Micro & Nanosystems, D-MAVT* Tactile Sensing With Scalable Capacitive Sensor Networks on Flexible Substrates
	Maximilian E. Merkel, *Materials Theory, D-MATL* Understanding Strongly Correlated Materials for the Electronics of the Future
	Sophie Marie Koch, *Wood Materials Science, D-BAUG* Wood-Templated Cellulose-Gelatine Composites for Biomedical Applications
	Ihor Cherniukh, *Functional Inorganic Materials, D-CHAB* Perovskite-Type Nanocrystal Superlattices From Lead Halide Perovskite Nanocubes
	Andrea Testa, *Soft & Living Materials, D-MATL* Biomimetic Active Droplets via Enzymatically Driven Reactions
	MaP Mastermind Quiz #2
14.15	**Flash Poster Presentations**
14.30	*Break*
Session 3: co-chaired by **Maksym Yarema** (*D-ITET*) & **Olivier Enger** (*BASF*)	
14.40	**Zhiyuan Zhang,** *Acoustic Robotics & Systems, D-MAVT* Microswarms Rolling in Acoustic Virtual Walls
	Fabio L. Bargardi, *Complex Materials, D-MATL* Driving Towards Sustainable Mobility: Manufacturing of Integrated Li-Ion Electrodes
	Alessia Villois, *Microfluidics & Nanoscale Science, D-CHAB* A Temperature-Controlled Droplet-Based Microfluidic Reactor for Kinetics of Protein Unfolding
	Christopher Dreimol, *Wood Materials Science, D-BAUG* Laser-Induced Graphitization on Temperature Sensitive Substrates
	Alba Sicher, *Soft & Living Materials, D-MATL* Structural Color From Solid-State Polymerization-Induced Phase Separation
	MaP Mastermind Quiz #3
15.50	**Thematic Group Discussions**
16.30	*Break*
16.40	**Award Ceremony** Art of Science Contest, MaP Image Contest, MaP Poster Prize, People's Choice Poster Prize, MaP Mastermind 2021
17.00	**Closing**
17.10	End of Symposium Day 2

Online Symposium – Special Instructions

This year's MaP Graduate Symposium is held on **ZOOM** at https://ethz.zoom.us/j/69349869234. For two program elements, the poster session and the social gathering, we meet on **Gather.town** at https://gather.town/i/wWh6fMst. Please be aware of having only one or the other active to avoid technical issues (e.g. acoustic feedback).

Gather.town

Gather.town is a 2D replica of real spaces with 8-bit graphics. It is supported on Chrome, Firefox and Desktop Safari (in Beta) and is optimised for computer devices (as opposed to mobiles or tablets). To enjoy audio and video exchange with other participants, please allow the program to access your camera and microphone. When entering Gather.town, please enter your full name (first + last name, in upper and lower case writing). You can move your avatar freely using the arrows of your computer keyboard. When avatars approach one another, participants can talk to each other through an automatically launched video call. If you should find yourself in a hot spot with many people, you might like to reduce your interaction distance with other avatars with the «quiet mode». Interactive objects such as posters and images can be entered for full-screen view by pressing the «x» key when your avatar is near the object. The private space near a poster allows to interact with the poster presenter and other attendees inside the space, while attendees outside the space are not interrupted.

For the symposium, we created the following dedicated spaces: The posters are located in two rooms, «Posters 1-29» and «Posters 30-57» (please find the list of posters on pages 20-22 in this booklet). For the social gathering, we will meet in the «Lounge». The images of the Image Contest are distributed across the Gather.town environment. To vote for your favourite poster, please visit one of the two votings booths in one of the poster rooms.
If you should require assistance, please visit the helpdesk in the main room.

Additional Instructions for poster presenters

During the live poster session (14 June, 15.45-16.45), you are kindly asked to stand in the shaded square in front of your poster. This shaded square is known as a «private space» and your audio/video will be shared with everyone else in this square, but not neighbouring spaces. Please consider using the pointer, allowing you to easily refer to a particular point of your poster. Gather.town is already set up – please feel free to visit the space already now to familiarise yourself with the platform.

Final Remark

Whether for ZOOM, Gather.town, to participate in the quizzes (slido) or take part in the votings (Google forms; here, a google account is required), please always indicate your full name (first + last name), written in upper and lower case letters, e.g. Sophie Matter.

Abstracts of Talks

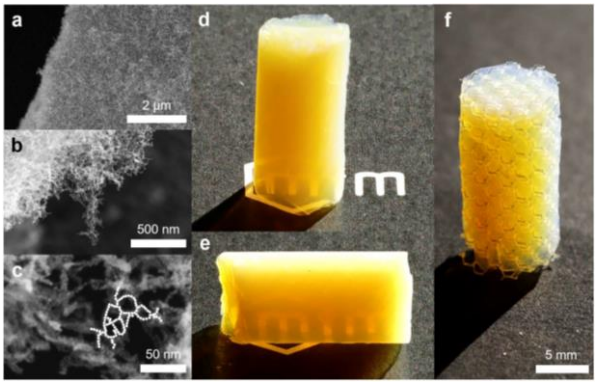
Session I: 14 June 2021, 13.15 – 14.25

Co-chaired by Daniel Ahmed (D-MAVT) & Pernilla Andersson (Sensirion)

How 3D Printed Polymeric Scaffolds Influence Geometry, Mechanical Stability and Photocatalytic Performance of Nanoparticle-based Aerogels

Murielle Schreck, Nicole Kleger and Markus Niederberger
Multifunctional Materials, D-MATL, ETH Zurich

Monolithic aerogels composed of crystalline nanoparticles have the great advantage that photocatalytic gas phase reactions can be carried out in three dimensions. At the same time, however, such aerogels suffer from low mechanical stability and it is difficult to produce them with complex geometries that are optimal for photocatalysis. Here, we report how we take control of the geometry of the photocatalyst by introducing carefully designed 3D printed polymeric scaffolds into the aerogels. Thanks to these scaffolds, we are able to systematically investigate and optimize fundamental parameters in gas phase photocatalysis such as the gas flow through the aerogel, the UV light penetration into the aerogel and the optimal geometrical fit with our customized continuous gas flow reactor to maximize the hydrogen production rate. By modifying the geometry of the aerogels, hydrogen production by photocatalytic methanol reforming is increased by almost a factor of three from 400 µmol g-1 h-1 to 1200 µmol g-1 h-1. Additionally, the rigid scaffolds enhance the mechanical stability of the fragile aerogels, lowering the number of rejects during synthesis. The combination of nanoparticle-based aerogels with 3D-printed polymeric scaffolds opens up a large number of unique opportunities to customize the geometry of photocatalysts for both the photocatalytic reactions as well as for the reactors to maximize the overall performance.



(a,b,c) SEM images of TiO_2-Pd aerogels at different magnifications and photographs of translucent cm-sized aerogels without (d,e) and with (f) an embedded 3D printed polymeric scaffold.

Towards a Golgi on a chip

Florin N. Isenrich[1], Marie-Estelle Losfeld [2], Markus Aebi[2] and Andrew J. deMello[1]
[1] Microfluidics & Nanoscale Science, D-CHAB, ETH Zurich
[2] Microbial Glycobiology, D-BIOL, ETH Zurich

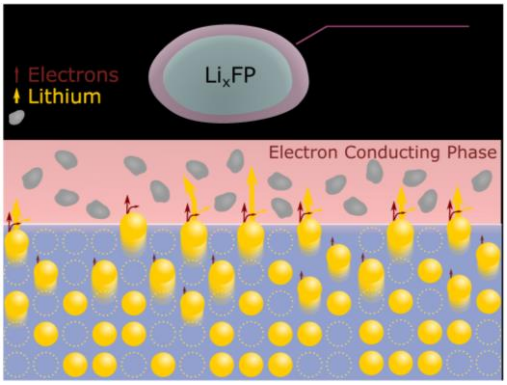
Protein glycosylation is a highly conserved process in eukaryotes. It changes the surface of proteins and is thus intimately involved in processes such as cell-cell recognition, antibody binding and recognition, and protein quality control. Protein glycosylation is not template driven - copies of the same protein in the same cell can possess different glycan forms.

The resulting glycosylation profile differs depending on the organism, organ, tissue, cell type and age. This poses a major issue in the production and approval of recombinant protein therapeutics. In order to improve glycoengineering in vivo a deeper understanding of the complex enzymatic processes is required.
Martin et al. developed a digital microfluidic chip capable of sulfonating heparan sulfate.[1] But, the chemical immobilization of the substrate and the low throughput limit the use of this device. However, no literature was found that investigates N-glycan glycoprotein modification using microfluidics.
We developed a droplet-based microfluidic platform that comprises prolonged incubation times with over 80 µl volume on-chip and picoinjection that enables sequential enzymatic reactions. We employ early enzymes of the glycosylation machinery, previously investigated by the Aebi group, to test our microfluidic platform.[2]
Preliminary results suggested adsorption of our low concentration enzyme to PDMS, impairing the enzymatic reaction. Non-specific adsorption of proteins to PMDS is a known phenomenon and surface modification is commonly used to reduce it.[3] To develop a system that can be used for a wide range of different proteins, we established our platform with a PTFE-based material. On it, we modified the N-linked glycans of our model protein ER-PDI and showed the successful incorporation and incubation of a second enzymatic reaction after picoinjection on-chip.
[1] J. G. Martin, et al., JACS, 131, 11041 (2009)
[2] C. Mathew, Diss. ETH. No. 25624 (2018)
[3] A. Gökaltun, et al., Sci. Rep., 9, 7277 (2019)

Controlling Li lithium ion battery (de)intercalation dynamics through interface design

Peter Benedek[1], Xueyan Zhao[1], Annina Moser[1], Ola Forslund[2], Nami Matsubara[2], Elisabetta Nocerino[2], Marisa Medarde[3], Yasmine Sassa[2], Ramesh Shunmugasundaram[1], Fanni Jurànyi[3], Martin Mansson[2] and Vanessa Wood [1]
[1] Materials & Device Engineering, D-ITET, ETH Zurich
[2] Department of Physics, KTH Stockholm
[3] Laboratory of Neutron Scattering, PSI

To achieve long-lasting, high performance lithium ion batteries, local inhomogeneous currents must be avoided. One driver of such inhomogeneity is the spinodal decomposition of active materials into Li rich and Li poor phases during charge and discharge. Whether such phase separation occurs is linked to the dynamics of lithium at the active material surface and within its bulk. Here, we show that surface coatings can be rationally designed to inhibit phase separation while not impacting the cycling rate performance.
Taking $LiFePO_4$ as a model system, we combine molecular modelling with muon spin spectroscopy and impedance spectroscopy to understand how different coatings impact surface electronic structure and Li dynamics. Operando x-ray diffraction is then used to confirm that phase separation can be mitigated via (i) locally slowing Li diffusion and (ii) decoupling electronic and ionic motion. Our results underpin the importance of characterizing electronic and ionic transport at battery interfaces to achieve better rate capability and battery life.

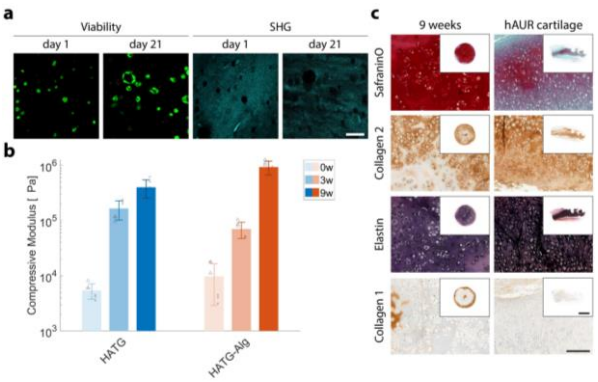


Schematic image of coated $LiFePO_4$ (LFP) particles. By studying the surface dynamics with different coatings, we can rationally design coating to suppress phase separation.

Formation of elastic cartilage in bioprinted auricles

Philipp Fisch[1], Killian Flégeau[1], Sergio Finkielsztein[2], Thomas Linder[3] and Marcy Zenobi-Wong[1]
[1] Tissue Engineering & Biofabrication, D-HEST, ETH Zurich
[2] Marine Polymer Technologies Inc. USA
[3] HNO Luzerner Kantonsspital

Bioprinting of functional tissue remains a major challenge as the process cannot reproduce the intricate complexity of native tissue and post-printing tissue maturation is required. This poses a particular problem for cartilage tissue engineering as the structure/composition-function relationship gives rise to the tissue's ability to sustain mechanical loads.
Recently we reported calcium-triggered enzymatic crosslinking (CTEC) bioprinting allowing us to bioprint enzymatically crosslinkable materials.[1] Such constructs were stable in vivo for 6 months and reached compressive moduli of up to 400 kPa. Through finetuning of our CTEC bioinks for auricular cartilage tissue engineering we were now able to generate constructs reaching up to 1MPa, approximately 2/3 of the compressive modulus of native human auricular cartilage. These constructs further showed a tissue composition comparable to human auricular cartilage in their elastin, glycosaminoglycan, collagen I and II composition (Figure).
By replicating auricular cartilage, we hope that the developed tissue can be used as an alternative treatment for patients born with microtia, a congenital malformation of the external ear. Thus, the current gold standard treatment, autologous costal cartilage repair, could be replaced with a less invasive treatment with a lower complication rate and without the risk of donor site morbidity.
[1] P Fisch, et. al., Adv. Funct. Mater. 31, 16 (2021).



(a) Viability and second harmonic generation (SHG). (b) Compressive modulus of the HATG and HATG-Alg Bioink after 0, 3 and 9 weeks. (c) Histology and immunohistochemistry of constructs after 9 weeks compared to human auricular cartilage.

Two-Level Compartmentalization for Triggered Reagent Delivery in Double Emulsions

Ariane Stucki[1], Petra Jusková[1], Nicola Nuti[1], Steven Schmitt[2] and Petra S. Dittrich[1]
[1] Bioanalytics, D-BSSE, ETH Zurich
[2] Bioprocess Laboratory, D-BSSE, ETH Zurich

abstract confidential

MaP Award 2021: 14 June 2021, 14.35 – 15.45

Chaired by André R. Studart (D-MATL, MaP Chair)

Tribological Insights into Shear Thickening Suspensions

Chiao-Peng Hsu
Soft Materials & Interfaces, D-MATL, ETH Zurich

Shear thickening is a ubiquitous rheological phenomenon whereby dense suspensions of particles in a fluid exhibit a viscosity increase at high shear. In this thesis, we focus on identifying the microscopic origins of discontinuous shear thickening in dense suspensions. The goal is to link the microscopic tribology at contact to the macroscopic rheological response. To this end, we utilize atomic force spectroscopy to characterize the friction and adhesion properties of model systems at the nanoscale, which we synthesize by bottom-up ap-proaches.

Smart Manufacturing of Curved Mass Timber Components by Self-Shaping

Philippe Grönquist
Wood Materials Science, D-BAUG, ETH Zurich

With the rise of free-form timber architecture enabled by recent developments in digital design and fabrica-tion, the demand for curved timber components is increasing. In this thesis, a novel approach for the manu-facturing of curved timber building components was proposed and analyzed. Following biological role models such as the bending of pine cone scales, a smart and efficient way to curve wood at large-scale is made pos-sible by the biomimetic concept of bi-layered laminated wood. This principle enables large programmed mate-rial deformations upon controlled moisture content change. The objectives of the thesis were to provide in-depth understanding of the mechanics of self-shaping wood bilayers and the up-scaling of the principle from the laboratory to the industrial scale in order to enable an application as form-stable curved elements for con-struction. The main challenges addressed were the accurate prediction of shape-change in terms of the natu-ral variability in wood material parameters, the scale-dependent impact of moisture gradients on mechanical behavior, and the influence of wood-specific time- and moisture-dependent deformation mechanisms during the shaping process. By using complex continuum-mechanical material models adapted to wood, the com-bined impact of these effects was characterized, and based on the gained insight, the up-scaling process to industrial manufacturing was successfully made possible. A collaborative project realized in 2019, the 14 m high Urbach tower, served as a proof of concept for both the application and the competitiveness of the novel developed biomimetic method for production of curved mass timber components.

Uniting Bioactivities in Hybrid Nanosystems for Wound Healing

Tino Matter
Nanoparticle Systems Engineering, D-MAVT, ETH Zurich

The advent of nanotechnology has given humanity a toolset to engineer materials with structural features one hundred thousand times smaller than the width of a

human hair. Especially when it comes to medicine and biology, nanotechnology offers an entirely new world of possibilities.

Fueled by such recent advances, this doctoral thesis presents novel inorganic nanomaterials for wound healing applications. Inorganic materials have several advantages over their organic counterparts, such as reproducibility, robustness, and lower production costs. To harness these benefits for a healthcare setting, however, high quantities of high-quality nanomaterials are required. One nanoparticle production technique that unites scalability with modularity, reproducibility, and a one-step synthesis is liquid-feed flame spray pyrolysis (LF-FSP). This method gives access to a wide spectrum of inorganic materials, of which bioactive metal oxides in particular have raised interest in the biomedical field.

In summary, this doctoral thesis shows how inorganic nanoparticle hybrids can be engineered by LF-FSP to serve as exogenous mediators of vastly complex biological processes, exemplified by the promotion of wound healing. Seemingly orthogonal bioactivities, such as toxicity against microbes and benignity towards mammalian cells, can be unified in a single nanoparticle hybrid system reminiscent of a Swiss army knife. Sophisticated nanoparticle compositions and architectures can be produced in a scalable and sterile single-step process, which eliminates many of the current roadblocks in the clinical translation of nanotherapeutics. The modularity and versatility of the concept of designing inorganic nanotherapeutics with direct, structure-dependent bioactivity offer great potential for manifold clinical applications beyond the field of wound healing.

Session II: 15 June 2021, 13.05 – 14.15

Co-chaired by Eleni Chatzi (D-BAUG) & Adelina Braun (Merck)

Tactile sensing with scalable capacitive sensor networks on flexible substrates

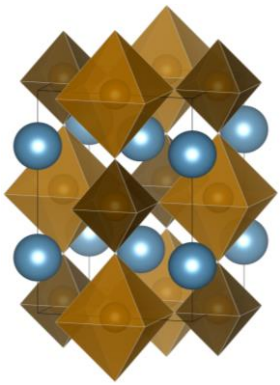
Johannes Weichart, Cosmin Roman and Christofer Hierold
Micro and Nanosystems, D-MAVT, ETH Zurich

abstract confidential

Understanding strongly correlated materials for the electronics of the future

Maximilian E. Merkel and Claude Ederer
Materials Theory, D-MATL, ETH Zurich

Materials with strong electronic correlations, i.e., strong effects due to the quantum nature of the electron-electron interaction, are potentially useful for various applications, such as data storage, transistors, or sensors. These applications try to exploit the sharp transition from metal to insulator that can occur in these materials, triggered by external influences such as strain, temperature, or applied voltage. For many strongly correlated materials, these metal-insulator transitions are also coupled to structural distortions, i.e., movements of the atoms of the crystal. However, simulating correlated-electron materials is a very challenging problem, which we tackle with a combination of density-functional theory and dynamical mean-field theory. Specifically, we address the example of $CaFeO_3$, which exhibits a metal-insulator transition close to room temperature. We show that the interplay between electronic repulsion and Hund's rule coupling in this material leads to charge disproportionation, where the nominal occupation of the Fe splits from Fe^{4+} into Fe^{5+} and Fe^{3+}, which then results in a drastic reduction of "free" electrons that can transport current. Furthermore, our computational method can quantitatively describe the strength of the structural distortion. Finally, we go beyond quantitatively describing the transition in $CaFeO_3$ and seek to elucidate the mechanism that mediates it.



The crystal structure of $CaFeO_3$ in its insulating state.

Wood-templated Cellulose-Gelatine Composites for Biomedical Applications

Sophie Marie Koch, Christian Goldhahn and Ingo Burgert
Wood Materials Science, D-BAUG, ETH Zurich & Cellulose and Wood Materials, Empa

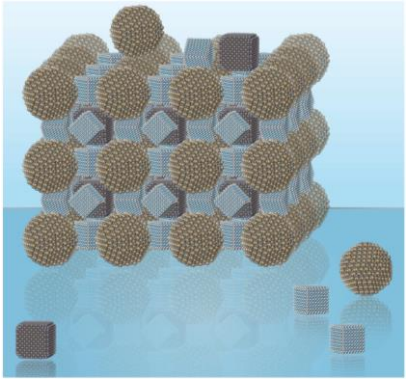
abstract confidential

Perovskite-type Nanocrystal Superlattices from Lead Halide Perovskite Nanocubes

Ihor Cherniukh[1,2], Gabriele Rainò[1,2], Thilo Stöferle[3], Max Burian[4], Alex Travesset[5], Denys Naumenko[6], Heinz Amenitsch[6], Rolf Erni[7], Rainer F. Mahrt[3], Maryna I. Bodnarchuk[1,2] and Maksym V. Kovalenko[1,2]
[1] Functional Inorganic Materials, D-CHAB, ETH Zurich
[2] Laboratory of Thin Films and Photovoltaics, Empa
[3] IBM Research Zurich
[4] Swiss Light Source, PSI
[5] Department of Physics and Astronomy, Iowa State University and Ames Lab
[6] Institute of Inorganic Chemistry, Graz University of Technology
[7] Electron Microscopy Center, Empa

Caesium lead halide perovskite nanocrystals, owing to high oscillator strength of bright triplet excitons, slow dephasing and minimal inhomogeneous broadening of emission lines, are promising building blocks for creating superlattice structures that exhibit collective phenomena in their optical spectra. Thus far, only single-component superlattices with the simple cubic packing have been devised from these novel nanocrystals, which have been shown to exhibit superfluorescence – a collective emission resulting in a burst of photons with ultrafast radiative decay (ca. 20 ps) that could be tailored for use in ultrabright (quantum) light sources[1]. However, far broader structural engineerability of superlattices, required for programmable tuning of the collective emission and for building a theoretical framework can be envisioned from the recent advancements in colloidal science[2]. We show that co-assembly of cubic and spherical steric-stabilized nanocrystals is experimentally possible and that the cubic shape of perovskite nanocrystals leads to a vastly different outcome compared to all-spherical systems. We present perovskite-type (ABO_3) binary nanocrystal superlattices, besides expected NaCl-type or common AlB2-type superlattices. In binary ABO_3 superlattices, larger spherical nanocrystals occupy the A sites and smaller cubic $CsPbBr_3$ nanocrystals reside on B and O sites. The deformability of ligand shell on cube corners makes the lattice stable over broad nanocrystal size ratio range. Targeted substitution of B-site nanocubes by truncated cuboid PbS nanocrystals leads to the exclusive formation of ternary ABO_3 superlattice (Fig.). All synthesized superlattices exhibit a high degree of orientational ordering of the $CsPbBr_3$ nanocubes. We also demonstrate the effect of superlattice structure on superfluorescent behaviour. Our work paves the way for further exploration of complex, ordered and functionally useful perovskite mesostructures.

[1] G. Rainò, et al., Nature 563, 671-675 (2018).
[2] M.A. Boles, et al., Chem. Rev. 116, 11220-11289 (2016).



Schematic representation of the ternary perovskite-type ABO_3 superlattice comprising spherical, truncated cuboid and cubic NCs.

Biomimetic Active Droplets via Enzymatically Driven Reactions

Andrea Testa[1], Mirco Dindo[2], Aleksander Rebane[1], Robert Style[1], Paola Laurino[2] and Eric Dufresne[1].
[1] Soft & Living Materials, D-MATL, ETH Zurich.
[2] Protein Engineering and Evolution Unit, Okinawa Institute of Science and Technology (OIST)

abstract confidential

Session III: 16 June 2021, 14.40 – 15.50

Co-chaired by Maksym Yarema (D-ITET) & Olivier Enger (BASF)

Microswarms Rolling in Acoustic Virtual Walls

Zhiyuan Zhang and Daniel Ahmed
Acoustic Robotics & Systems Lab, D-MAVT, ETH Zurich

Micro- and nanorobotics could become a powerful tool that would allow specialized tasks in medicine, including non-invasive surgical procedures and drug delivery to hard-to-reach sites. However, manipulation at the microscale is challenging, typically requiring a nonreciprocal movement of the robot to propel. An alternate and widely used manipulation strategy is rolling; however, the concept is restricted to the walls or boundary conditions. Here, we demonstrate microswarms rolling in mid-liquid for the first time in the absence of any walls by combining acoustic and magnetic fields. Pressure nodes of the acoustic standing wave field mimic the virtual walls. The rotating magnetic field was employed to self-assemble and rotate the superparamagnetic microswarms. By switching the acoustic virtual wall pattern and the magnetic field rotational direction, we achieved the microswarm manipulation in arbitrary acoustic virtual walls to draw the "E", "T", and "H" letters, without the limitation of any surface or boundary conditions. The newly presented microswarm manipulation strategy will provide an exciting transport and delivery technique to science and engineering disciplines.

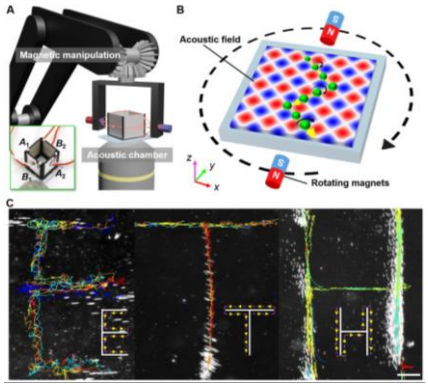


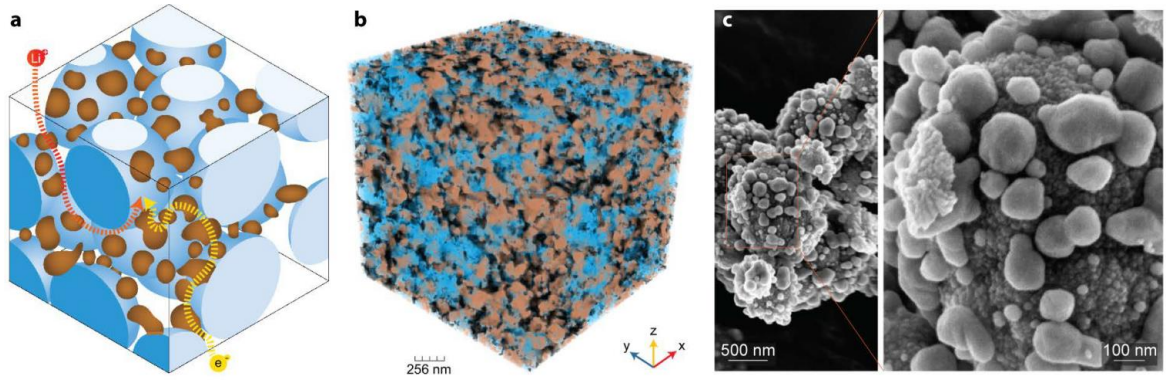
Illustration of microswarms rolling in acoustic virtual walls. (A) The experimental setup consists of the magnetic effector held and rotated by the robotic arm and the acoustic chamber mounted on the inverted microscope. The insert shows details of the acoustic chamber. (B) Microswarms exhibit rolling-like motion in the combined two-dimensional acoustic standing wave field and the rotating magnetic field. (C) Microswarms write the word “ETH” by the tracked trajectory. Scale bar, 100 μm.

Driving towards sustainable mobility: manufacturing of integrated Li-ion electrodes

Fabio L. Bargardi[1], Juliette Billaud[2], Claire Villevieille[2], Florian Bouville[1,3] and André R. Studart[1]
[1] Complex Materials, D-MATL, ETH Zurich
[2] Electrochemical Laboratory, PSI
[3] Centre for Advanced Structural Ceramics, Imperial College London

Transportation is responsible for 14% of 2010 global greenhouse gas emissions. This energy demand is covered by fossil fuels burned for road, rail, air and marine transportation. Almost 95% of the fuels derives from non-renewable petroleum-based fuels[1]. Technological development has enabled alternatives to fossil fuels for the private mobility, e.g. batteries for electric cars.
Topic of this talk will be the demonstration of a successful strategy to enhance the performance and increase energy density of lithium-ion-battery cells through the design of an optimized microstructure.

Minimization of electronic and ionic transport limitations is achieved by promoting electrical conductivity and mechanical stability through a three-dimensional copper network within the electrode [2].
Through the fabrication of an architectured electrode we show that it is possible to increase the amount of active material and reduce the mass of additives and packaging. Here, we demonstrate a simple processing route in which Cu-coated ZnO powders are uniaxially pressed into the final electrode shape. Our highly loaded integrated anodes display a volumetric charge capacity 6–10 fold higher than Cu-free ZnO films.
[1] Climate Change 2014: Mitigation of Climate Change, Cambridge University Press, ISBN: 9781107654815 (2015).
[2] Bargardi et al., Scientific Reports 10, 12401 (2020).



(a) Schematics of the tri-continuous interpenetrating network of ZnO (blue), Cu (brown) and pore phases (transparent) obtained upon uniaxial pressing of the architectured powder, (b) 3D reconstruction of the interpenetrating phases of a pressed electrode, (c) SEM image of Cu-coated ZnO particles[2].

A temperature-controlled droplet-based microfluidic reactor for kinetics of protein unfolding

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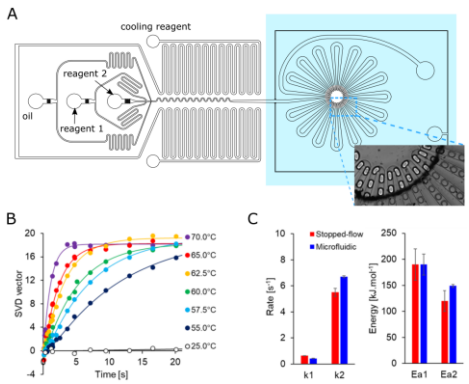
Several biochemical studies involve the investigation of rapid reactions. Often, important information about these processes can be obtained by acquiring time-resolved data at different temperatures. The rapid mixing of reagents to minimize the reaction dead time and accurate temperature control are crucial. To address these aspects, we show a simple microfluidic platform for measuring protein unfolding kinetics with accurate temperature control, with a time resolution ranging from a few milliseconds to 30 seconds. We used deep-UV illumination to achieve direct excitation of intrinsic fluorophores, eliminating the need for extrinsic labels. We used a spectrophotometer for fluorescence detection, to obtain highly informative full spectra as output.
We investigated the unfolding kinetics of the LinB enzyme as a function of temperature. Afterwards, we extracted kinetic and thermodynamic information and we compared it with the results from a commercial T-jump/stopped-flow apparatus. We found excellent agreement between the two techniques. Moreover, the full spectra obtained from microfluidics allowed the unambiguous identification of the individual unfolding steps, which could not be distinguished with the stopped-flow data.
Therefore, our microfluidic platform can be used to probe protein unfolding and other rapid biomolecular reactions, especially when limited sample quantities are available and high-throughput multi-temperature screening is required.



(A) Microfluidic chip design including a flow focusing droplet generator, a winding channel for efficient mixing and a reaction/heating loop. The blue area indicates the heating zone. Insert: images of droplet distribution in the reaction loop under bright field.)B) Unfolding kinetics of LinB measured with the microfluidic device. SVD amplitude vectors calculated from the time-resolved spectra at different temperatures (each SVD data point represents a whole spectrum). The solid line represents the best global fit to the SVD amplitude vectors. (C) The comparison of the rate constants and thermodynamic parameters obtained by stopped flow (red) and microfluidic (blue) analysis (reference temperature 338.15 K). The error bars represent the standard errors of nonlinear fit to the stopped-flow data and standard errors estimated during global fit for microfluidic data.

Laser-induced graphitization on temperature sensitive substrates

Christopher Dreimol Guido Panzarasa and Ingo Burgert
Wood Materials Science, D-BAUG, ETH Zurich & Cellulose and Wood Materials, Empa

Electronic waste (E-waste) is a huge concern all over the world, as one of the fastest growing waste streams in terms of both volume and environmental impact. Direct writing of laser-induced graphene (LIG) conductive patterns on biological substrates, and especially on wood, is a promising strategy to promote the development of environmentally friendly and sustainable electronics. However, the large-scale manufacturing of high quality conductive patterns remains challenging due to the complex nature of the surface of wood (inhomogeneous structure with variable chemical composition). Moreover, factors such as high ablation rates, the need of multiple lasing steps and the use of fire retardants are also limiting the applicability of conventional laser processes for the production of sustainable electronic devices. Here, we demonstrate a novel route for direct laser writing of LIG on wood and wood-derived materials (e.g. wood, paper). Our approach, which combines a fast CO_2-laser treatment in normal atmosphere with a simple chemical pre-treatment of wood, allows obtaining highly conductive surfaces on wood and wood-derived materials with unprecedented efficiency at large scale.

Structural Color From Solid-State Polymerization-Induced Phase Separation

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Structural color is produced by nanostructures able to provide a variation in the material refractive index on the order of the wavelengths of visible light. These structures can cancel, deflect or reinforce specific wavelength ranges, generating a permanent, very bright, non-fading color with no need of pigments or dyes.

Many natural materials display structural color, which is developed through self-assembly and phase separation[1,2]. However, most synthetic structural colors are produced in a two-step process involving the sequential synthesis and assembly of building blocks[3].

Inspired by the formation through phase separation of the quasi-ordered photonic structures in the feathers of many birds[1,4], we developed a self-limiting approach to polymerization-induced phase separation that can produce stable structures at optical length scales. The resulting composites have a blue or white color. We also demonstrate the flexibility of this approach by producing structural color in filaments and large sheets.

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[3] G. Shang, M. Eich, and A. Petrov. APL photonics 5.6 (2020): 060901.
[4] V. Saranathan, et al., Journal of The Royal Society Interface 9, 2563 (2012).

Abstracts of Posters

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1 Küffner, Andreas

Bioinspired liquid-liquid phase separation for reactive materials

Andreas M. Küffner, Lenka Faltova and Paolo Arosio
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Spontaneous liquid demixing (LLPS) of biomolecules appears to be an efficient strategy developed by cells to organize reactions in space and time. This process allows cells to modulate biochemical reactions by locally changing the concentration and the environment of specific components. Here, we developed a strategy to couple the formation of biomolecular liquid compartments with reactions occurring within them[1]. For this we fused liquid liquid demixing peptides, so called low complexity domains, with globular and functional domains. We studied the influence of different LCDs on the LLPS of fusion proteins and applied the gained knowledge to engineer our formed microreactors[2]. Subsequently, we show that these micro-reactors are characterized by a polarity comparable to methanol which promotes recruitment of small molecules. Despite exhibiting higher viscosity with respect to the surrounding solution, the reactors are liquid-like and allow molecular diffusion within their interior. We demonstrate that the local increase in enzyme concentration accelerates the corresponding enzymatic rate[3]. Additionally, we investigated the effect of the microreactor environment on a polymerisation reaction using the fibrillation of aβ-42 peptide and demonstrate the inhibition of this reaction[4]. This flexible strategy enables the generation of biomolecular micro-reactors with modulated reactivity, with potential applications in heterogeneous biocatalysis or biologics formulation.

[1] L. Faltova, A. M. Küffner, et. al., ACS Nano 12, 9991-9999 (2018).
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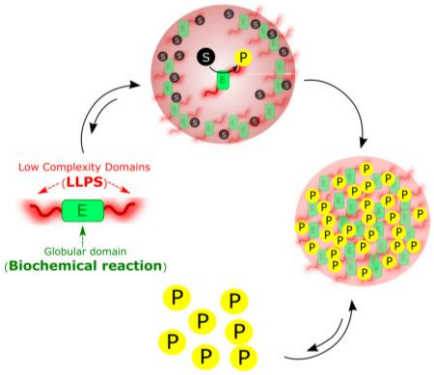
[3] A. M. Küffner, et. al., ChemSystemsChem 2, e2000001 (2020).
[4] A. M. Küffner, et. al., Chem. Sci. 12, 4373-4382 (2021).



Schematic depicting the catalytic reaction in the presence of biomolecular microreactors.

2 Ding, Yong

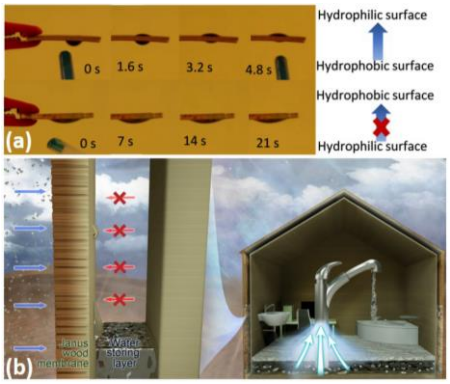
Janus wood membranes for autonomous water transport

Yong Ding, Kunkun Tu, Ingo Burgert and Tobias Keplinger
Wood Materials Science, D-BAUG, ETH Zurich & Cellulose and Wood Materials, Empa

Autonomous and directional transport of liquids is crucial for many applications, ranging from microreactors to water harvesting. Particularly, Janus membranes, with asymmetric wettability on two sides, represent enticing opportunities to address this challenge. With the inner driving force arising from

the asymmetric wettability, Janus membranes can promote the desired transport without external energy input[1]. However, elaborate bottom-up fabrication processes and poor mechanical performance of commonly employed membrane substrates often restrict their utilization, especially for engineering applications. Here we report a wood-based Janus membrane demonstrating directional, spontaneous, fast transport of water[2]. Profiting of woods unique intrinsic porous structure, wood serves as an ideal substrate for liquid transport. Native wood membranes were first hydrophobized by fluoro oxysilane/TiO_2 nanoparticles, and then UV-irradiated on one side to create the needed wettability gradient through the thickness of Janus wood membrane. Mechanically robust bio-based and renewable Janus wood membranes represent a crucial milestone towards larger-scale application of Janus membranes, for example in bilayer structures with excellent fog-capturing efficiency implemented in future smart building applications.

[1] H. Yang, et al., Adv. Mater. 30.43 (2018).
[2] Y. Ding, et al., J. Mater. Chem. A 8.42 (2020).



(a) Anti-gravity directional water transport by Janus wood membrane and (b) its application in fog collection.

3 Pioli, Roberto

Capillary deposition of microorganisms for the study of cells in spatially controlled environments

Roberto Pioli[1], Miguel Angel Fernandez Rodriguez[2,3], Fabio Grillo[2], Laura Alvarez[2], Roman Stocker[1], Lucio Isa[2] and Eleonora Secchi[1]
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[3] Laboratory of Surface and Interface Physics, Biocolloid and Fluid Physics Group, Faculty of Sciences, University of Granada

Controlled and precise deposition of microorganisms into defined spatial arrangements offers unique and innovative possibilities for the study of microbial physiology and interactions. Full control over the geometrical arrangement is highly desirable due to the crucial importance of distances in microbe-microbe interactions, arising from their dependence on the propagation of chemical signals. Coupling accurate spatial patterning and full control over environmental conditions would provide a powerful and versatile platform for single-cell studies in microbial ecology. To this end, we have developed a microfluidic platform to extend a capillary deposition technique originally designed for colloidal particles, called sCAPA[1,2] (sequential capillarity-assisted particle assembly), to bacterial systems. This technology exploits the capillary forces[3] resulting from the controlled motion of an evaporating droplet inside a microfluidic channel to capture individual particles[4] or microorganisms in an array of traps microfabricated onto the substrate. Sequential depositions allow the generation of the desired spatial

layout of single or multiple microorganisms. We successfully calibrated this new technique on colloidal particles[4] and tested it on bacteria. In our platform, the coupling of single-cell deposition and microfluidic technology allows both geometric patterning and precise control of environmental conditions, and thus opens up a window into the physiology of single microbes and the ecology of microbe-microbe interactions, as shown by preliminary experiments.

[1] Ni, S., Leeman, J., Wolf, H. & Isa, L., Faraday Discuss. 181, 225-242 (2014).
[2] Isa, L., Kumar, K., Muller, M., Grolig, J., ACS Nano 4, 5665-5670 (2010).
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4 Böcker, Lukas

Interplay of interfacial stabilisation and extract efficiency of microalgae proteins

Lukas Böcker[1], Pascal Bertsch[2], Severin Eder[3], Jotam Bergfreund[2], Peter Fischer[2] and Alexander Mathys [1]
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[2] Food Process Engineering, D-HEST, ETH Zurich
[3] Food Biochemistry, D-HEST, ETH Zurich

Microalgae gain increasing importance as alternative protein source for food production and biotechnological systems. Their protein-content of up to 70% bears potential for multiple functional applications in the food, nutraceutical and cosmetics industries. This potential coupled with microalgae's ability to be grown on non-arable land and to fixate CO_2 when cultivated photoautotrophically, motivates the foreseen impact on major challenges of the sustainable development goals. Economic constraints and a low technical readiness level impede large scale applications of their bulk proteins, so far. Thus, isolates from Arthrospira platensis were investigated to stabilize fluid interfaces in order to utilize such high value fractions in a cascading way following biorefinery principles.
Spray-dried A. platensis, commonly named Spirulina, were disrupted by high-pressure homogenization. Soluble components were separated by centrifugation prior to precipitating proteins at their overall isoelectric point. Resuspended precipitate was diafiltrated with a molecular weight cut off of 5'000 kDa. Extracts at all different purification steps were tested for their ability to stabilize interfaces and emulsions. Model emulsions prepared by high pressure homogenization were characterized by bubble size distribution over time and creaming height. Interfacial stabilization was assessed with bubble pressure tensiometry and interfacial oscillatory shear rheology.
Stabile emulsions could be formed with all different extracts. If normalized for protein concentration, mean bubble size decreased with purification from crude microalgae extracts to protein isolates. This was underscored with differences in building up an interfacial viscoelastic network at the oil-water interface in the rheological measurements. Protein isolates directly established a viscoelastic network whereas soluble extracts depicted a lag-phase reasoned with a dominant influence of small molecular weight surfactants.
Results emphasize the crucial impact of proteins in stabilizing fluid-fluid interfaces highlighting its capabilities for the food and cosmetics industry. Simultaneously, a balance must be struck between purification and extraction efficiency to optimally employ microalgae proteins.

5 Bader, Johannes

Loading of Nucleic Acids into Extracellular Vesicles – What is Possible?
Johannes Bader and Jean-Christophe Leroux
Drug Formulation & Delivery, D-CHAB, ETH Zurich

Extracellular vesicles (EVs) are believed to usher in a new era in the field of nanomedicine. These intercellular communicators consist in heterogeneous populations of cell-secreted vesicles originating from endosomes (i.e., exosomes) or bud from cellular membranes (i.e., microvesicles). Their involvement in many physiological and pathological processes make them promising candidates for biomarker applications in liquid biopsies, as well as biocompatible nanocarriers for drug delivery purposes [1]. A challenge in EV-mediated drug delivery is the efficient encapsulation of highly charged macromolecules, such as nucleic acids. In this study, EVs derived from bone marrow stromal cells were used to investigate different exogenous loading techniques. The production of EVs was scaled up by employing 3D cell culture on microcarriers to expedite the manufacturing process. Physicochemical properties and characteristic EV markers were analyzed according to standard guidelines. An RNA aptameric sensor was employed as a tool to monitor RNA retention inside the aqueous vesicle core post-loading. The preliminary data point out that current techniques fail to entrap RNA inside EVs, with the exception of the commercially available Exo-Fect™ Exosome Transfection Reagent. Future research efforts will work towards validating previous findings and developing novel protocols to incorporate functional oligonucleotides into EVs, which will then be tested in vitro with cell-based assays.

[1] R. Kalluri, and V.S. LeBleu, Science 367, 6478 (2020).

Acknowledgment: This project received generous funding from Skintegrity.ch.

6 Dietsche, Claudius

Protein profiling of single immune-cell on a microfluidic device
Claudius L. Dietsche, Elisabeth Hirth and Petra S. Dittrich
Bioanalytics, D-BSSE, ETH Zurich

abstract confidential

7 Lee, Seunghun S.

Silicon Nitride, A Bioceramic for Bone Tissue Engineering: A Reinforced Cryogel System with Antibacterial and Osteogenic Effects
Seunghun S. Lee[1], Leanid Laganenka[2], Xiaoyu Du[1], Wolf-Dietrich Hardt[2] and Stephen J. Ferguson[1]
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[2] Institute of Microbiology, D-BIOL, ETH Zurich

Silicon nitride (SiN, [Si_3N_4]) is a promising bioceramic for use in a wide variety of orthopedic applications. Over the past decades, it has been mainly used in industrial applications such as the space shuttle engines, but not in the medical field due to scarce data on the biological effect of SiN. More recently it has been increasingly identified as an emerging material for orthopaedic implant applications. Although a few reports about antibacterial property and osteoconductivity of SiN have been published, to date, there have been limited studies of SiN-based scaffolds for bone tissue engineering. Here, we developed

a silicon nitride reinforced gelatin/chitosan cryogel system (SiN-GC) by loading SiN microparticles into a gelatin/chitosan cryogel (GC), with the aim to produce a biomimetic scaffold with antibacterial and osteogenic properties. In this scaffold system, the GC component provides a hydrophilic and macroporous environment for cells while the SiN component not only provides antibacterial properties and osteoconductivity, but also increases the mechanical strength of the scaffold, to provide enhanced mechanical support for the defect area and a better osteogenic environment. First, we analyzed characteristics of SiN-GC with different SiN concentrations, such as interconnected porosity, mechanical properties and swelling ratio, then we checked apatite forming capacity in simulated body fluid and protein adsorption capacity. Next, we started in vitro experiments and confirmed an antibacterial effect of SiN-GC against E. coli and S. aureus and enhanced cell proliferation, mineralization and osteogenic gene upregulation for pre-osteoblast cells. Finally, we developed a bioreactor to culture cell-laden scaffolds under cyclic loading to mimic physiological conditions and were able to demonstrate improved mineralization and osteogenesis from SiN-GC. Overall, we confirmed the antibacterial and osteogenic effect of a SiN-GC and the results indicate that silicon nitride has a promising potential to be developed further for bone tissue engineering applications.

8 Kamml, Julia

Advanced Glycation End-Products leading to inferior material properties in collagen

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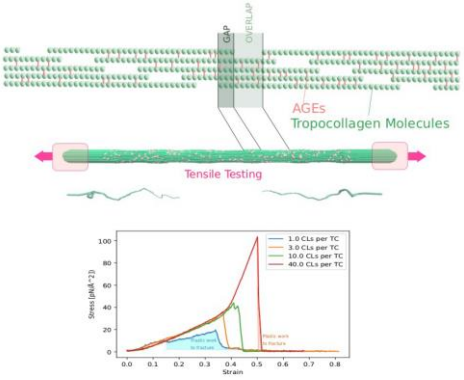
[2] School of Civil and Environmental Engineering, Cornell University

Collagen fibrils are the main building constituent of bone. Their staggered building pattern with crosslinks connecting tropocollagen molecules to a fibril provides them with astonishing mechanical properties: high elasticity, large strength and a substantial energy dissipation during deformation. It has been observed that the augmented glycation level in diabetic patients triggers an increased formation of random non-enzymatic crosslinks, so-called Advanced-Glycation-Endproducts (AGEs) between tropocollagen molecules.
Our study aims to reveal the mechanisms leading to inferior bone quality in diabetic patients using a computational bottom-up approach. In a first step, we implemented a 3D coarse-grained model of a collagen fibril segment presenting five repeating gap- and overlap zones, the basic building unit of collagen fibrils. Longitudinal tensile tests applying Molecular Dynamics are performed until fracture, gradually increasing the amount of random cross-links in order to investigate the influence of the density of AGEs on the mechanical behavior.
We observe three different regimes in the stress-strain curves, depending on the amount of crosslinks. Further, the plastic work to fracture decreases with an increasing crosslink density. The next step is to identify the location where the fibril ruptures, whether it is crosslinks or tropocollagen molecules and whether this is dependent on the AGE crosslinking.



Tensile Tests on collagen fibrils with different AGEs densities - the crosslinks(pink) are randomly distributed between the tropocollagen molecules (green) in the collagen fibril segment, built with the typical gap and overlap zones in its geometry - Stress-strain-curves show 3 different regimes depending on the amount of AGEs in the fibril

Soft Materials

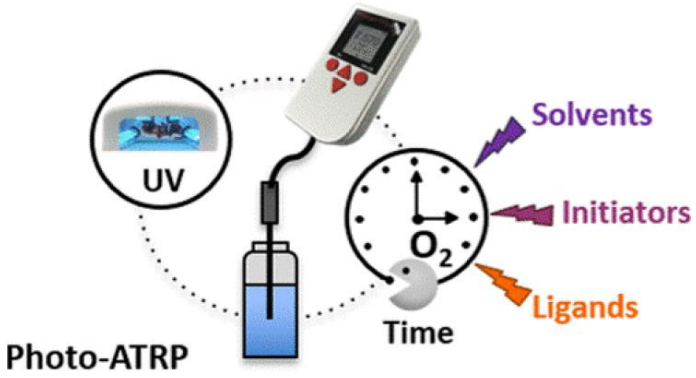
9 Rolland, Manon

Effect of Polymerization Components on Oxygen-Tolerant Photo-ATRP

Manon Rolland, Richard Whitfield, Daniel Messmer, Kostas Parkatzidis, Nghia P.Truong and Athina Anastasaki
Polymeric Materials, D-MATL, ETH Zurich

Photo-ATRP has recently emerged as a powerful technique that allows for oxygen-tolerant polymerizations and the preparation of polymers with low dispersity and high end-group fidelity. However, the effect of various photo-ATRP components on oxygen consumption and polymerization remains elusive. Herein, we employ an in situ oxygen probe and UV–vis spectroscopy to elucidate the effects of ligand, initiator, monomer, and solvent on oxygen consumption[1]. We found that the choice of photo-ATRP components significantly impacts the rate at which the oxygen is consumed and can subsequently affect both the polymerization time and the dispersity of the resulting polymer. Importantly, we discovered that using the inexpensive ligand TREN results in the fastest oxygen consumption and shortest polymerization time, even though no appreciable reduction of $CuBr_2$ is observed. This work provides insight into oxygen consumption in photo-ATRP and serves as a guideline to the judicious selection of photo-ATRP components for the preparation of well-defined polymers.

[1] Rolland, M.; Whitfield, R.; Messmer, D.; Parkatzidis, K.; Truong, N. P.; Anastasaki, A. Effect of Polymerization Components on Oxygen-Tolerant Photo-ATRP. ACS Macro Lett. 2019, 8 (12), 1546−1551.



Effect of ATRP components on oxygen consumption

10 Grob, Lucas

Filter-less Separation Technique for Micronized Anthropogenic Polymers from Artificial Seawater

Lucas Grob[1], Liridon Zeneli[1], Eileen Ott[1], Jacopo Vialetto[2], Jotam Bergfreund[1], Yasushi Takeda[1] and Erich J. Windhab[1]

[1] Food Process Engineering, D-HEST, ETH Zurich
[2] Soft Materials and Interfaces, D-MATL, ETH Zurich

Anthropogenic polymer particulates (APP) are a highly researched topic, from the identification of the different sources to their impact on living organisms, micronized anthropogenic polymers pose a threat to many ecosystems. Prevalently found are microplastic (MP) including PMMA. Additionally, micronized rubber powder (MRP), which originates from tire abrasion but also is used a filler material for various other products, can be found. Due their small size, less than 120 µm in diameter, and the relative low concentrations found in water, the foaming behavior of MRP and MP was investigated. Further, a simple, fast and filter-less technique was developed to remove APP from seawater. In a first step, we characterized the MRP and found two different particle behaviors, one fraction which forms clusters and was more prone to the air-water interface and the second fraction accumulating at the bottom. Both MP and MRP stabilized the foamed artificial seawater and MilliQ water, indicating a preferred localization of APP at the air-water interface. Thus, when added to a modified hydrocyclone (mHC) process with an additional defined bubble flow, an extraction ratio of 26% compared to without bubble flow of 3.7% was achieved. The mHC extracts and up-concentrates particles with densities similar to water with the use of their promotion of the air-water interface. These promising results show that this technique could be used in wastewater treatment plants to further purify water.

11 Parkatzidis, Kostas

Tailoring polymer dispersity by (PET)-RAFT polymerization: a versatile approach
Kostas Parkatzidis, Richard Whitfield and Athina Anastasaki
Polymeric Materials, D-MATL, ETH Zurich

Unlike natural biopolymers, such as DNA and proteins, synthetic polymers have a distribution of different molecular weight species. This distribution is measured by a dispersity value and has a significant influence on polymer properties. It is therefore highly beneficial to develop strategies to systematically tune the dispersity, but to date current methods have limitations in monomer scope, block co-polymer accessibility, and attainable dispersity range[1]. Here, we report a straightforward and versatile batch method based on reversible addition-fragmentation chain transfer (RAFT) polymerization to tailor the molecular weight distributions for a wide range of monomer classes, including acrylates, acrylamides, methacrylates, and styrene. In addition, our methodology is compatible with more challenging monomers, such as methacrylic acid, methyl vinyl ketone, and vinyl acetate. Control over dispersity is achieved by mixing two RAFT agents with sufficiently different chain-transfer activities in various ratios, affording polymers with monomodal molecular weight distributions[2]. Moreover, the present approach can be applied also in photo-induced electron/energy RAFT (PET-RAFT) polymerization. Benefits of the approach include the use of visible light irradiation, ppm concentrations of a photo-redox catalyst and the possibility to manipulate dispersity in the absence of external deoxygenation methodologies, which significantly simplify the process[3].

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12 Chen, Jia Lu

Thin Polymeric Materials and Processing Routes for Novel Biomedical Implants

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abstract confidential

13 Hofmann, Martin

Stretch, fold, and break: Intensification of emulsification of high viscosity ratio systems by fractal mixers

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During emulsification process design, the bulk and interfacial rheology of the target formulation must be carefully considered. Formulations with high viscosity ratios and/or finite interfacial elasticity are particularly challenging to emulsify, as conventional drop-breakup methods consume significant energy and provide limited control over polydispersity. Here, we develop a two-stage process that produces monodisperse emulsions from high viscosity ratio constituents. In the first stage, a custom static mixer generates co-flowing layers of alternate phases, and progressively thins layers until they rupture, thus forming a high-internal phase emulsion. The interfacial properties and flow conditions that promote stable fractal multiplication are discussed. In the second stage, extensional flow elements refine the polydispersity. We demonstrate the utility of this novel process by producing remarkably monodisperse polyisobutylene-in-water emulsions with an energy efficiency that is orders of magnitude higher than classical emulsification methods. The moderate throughputs achieved show promise for upscaling and intensification in industrial applications.

14 Renggli, Damian

Operation Windows for Interfacial Rheometry

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The interfacial rheology of liquid interfaces becomes important if surface active species such as surfactants, particles or proteins are present at the interface[1,2]. The broad interest in these complex interfaces covers topics from foam or emulsion stability to structural design in food or understanding the behavior of phospholipids as lung surfactants and is still an active area of research[3,4].
Confining soft matter to a fluid interface leads to thin monolayers of material, therefore resulting in a very weak mechanical response which might be insufficient to be measured accurately. This inherently soft response combines with other important challenges, including instrument inertia, sample inertia (momentum diffusion), subphase flow (Boussinesq limits), contact line imperfections, and alignment errors. In this work, we study this list of experimental challenges and derive equations for the operating limits of various macroscopic interfacial rheometers including the interfacial needle shear rheometer,

the double wall ring and the bi-cone geometries. We experimentally investigate the limitations defined intrinsically by the instrument as well as the ones emerging from the properties of the interface of interest. The results provide cautionary examples and guidelines for anyone measuring extremely soft materials[5].
We apply the operating windows to phospholipid monolayers at the water—oil interface. The monolayers consists of mixtures of saturated (palmitoyl) and unsaturated (oleoyl) phosphatidylcholines, which, in the shape of bilayers, form the cell membrane.

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15 Niggel, Vincent

Shaping the surface of silica particles by the competition between two silanes
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The synthesis of silica nanoparticles in a controlled and uniform way is easly achieved through the Ströber process[1]. However, such synthesis provides only smooth particles. In the last years, new synthesis protocols have been developped to engineer the roughness of silica particles, for example, by heterocoagulation[2]. Another promising route is the association of two different silanes, which, under special conditions, will create golf ball-like particles[3] with controlled morphology in a single reaction. Through this study, we perform an extensive screening of the ratio between the two silanes, TEOS and VTMS, and the concentration of ammonia in the suspension, to demonstrate the synthesis of different particles, whose surface was characterized by AFM. This approach enables the creation of large quantities of well-defined rough particles, e.g. as model systems in dense suspension rheology.

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Optics

16 Guo, Fangwei

Transparent antifogging CeO_2-x-TiO_2 - Xanthan gum composite coatings with self-healing and robust properties
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Fogging can significantly reduce the clarity of a transparent substrate, resulting in not only inconvenience but also potential safety risks, for instance the applications in windshield, eyeglass, camera lens, display device in medical analytical instrument. However, interface rough surfaces only a small fraction of the overall area is in contact with the liquid-experience high local pressures under mechanical load, making them fragile and highly susceptible to abrasion. Additionally, abrasion exposes

underlying materials and may change the local nature of the surface from hydrophobic to hydrophilic, resulting in the pinning of water droplets to the surface. Here we show that robust wet-style superhydrophobic coating can be realized by structuring surfaces at two different length scales, with a nanostructure design to provide a hydrophilic reservoir and a microstructure pattern design to provide durability by using a simply micro-printing stamp. The microstructure is an interconnected surface frame containing 'honeycomb pockets' that house super-hydrophilic and mechanically fragile nanostructures. This surface frame acts as 'armour', preventing the removal of the nanostructures by abradants that are larger than the frame size. The coatings comprise Xanthan gum, PVP and CeO2-x-TiO2 nanoparticles. The coatings showed smart intrinsic self-healing characteristics towards wounds caused by external forces, which is attributed to sufficient free hydroxyl groups at the scratched interfaces to reform H-bonds across the interfaces. All the unique characteristics of CeO2-x-TiO2-Xanthan gum composite coatings provide a promising method for self-healing, long-term antifogging, excellent mechanical property, high transmittance and large-scale feasibility.

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17 Marcato, Tommaso

Perovskite LEDs with Over 24% External Quantum Efficiency Using Outcoupling-Enhanced Colloidal 2D Nanocrystals

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Colloidal lead halide perovskites (LHPs) are an emerging class of light-emitting semiconductors that enables inexpensive roll-to-roll fabrication of ultra-color pure light-emitting diodes (LEDs) to advance the future display and illumination technologies. Hence, highly energy efficient and long-lasting perovskite LEDs are indispensable before their assimilation in commercial devices. Particularly, the performance of perovskite LEDs are strongly limited due to three crucial factors, including (i) low photoluminescence quantum efficiency (η_{PL}), (ii) poor charge carrier mobility, and (iii) low light-outcoupling efficiency (η_{out}). Thus, numerous efforts have been focused to enhance the η_{PL} in the colloidal LHP NCs. The η_{out} of LEDs can be estimated to <15% using classical optics principle, $\eta_{out} = 1/(2n^2)$, which is limited by the refractive index (n) of perovskite emission layer. However, the large fraction of trapped excitons opening-up a huge space for improvement in the η_{ext} of QD LEDs. Here, we demonstrate efficient, ultra-pure green EL based on colloidal two-dimensional (2D) superlattices by mixing the formamidinium into methylammonium lead bromide perovskites. We also propose a theoretical model to relate the anisotropic NC shape to the observed preferential horizontal orientation of the emission transition dipole moments even for weakly confined thick nanoplatelets. For our champion perovskite LED devices, comprising asymmetric 2D superlattices thin films with near-unity η_{PL}, show a highest external quantum efficiency (η_{ext}) of >24%. Thus, ultimately high performance in the quantum dot LEDs is attributed to high light-extraction efficiency (η_{out}) of >32% due to horizontal orientation of emission transition dipole moment in 2D superlattices and low refractive index carrier transporting layers. Moreover, the color gamut covers over 99% of Rec. 2020 standard in the CIE 1931 color space, respectively, representing the “greenest” LEDs ever reported. This is among the highest EL performance in all types of quantum dot LEDs ever reported by far.

18 Bobzien, Laric

Nanopatterning of Phase-Change Material Thin Films For Tunable Photonics

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For manipulation of light's amplitude, phase and polarization, metasurfaces arose as promising candidates with capabilities beyond those of classical optical components. Once fabricated, however, metasurfaces have set optical properties and are thus passive. Active metasurfaces are made out of nanostructures whose optical properties can be externally manipulated[2]. To tune e.g. the optical environment of the nanostructures, phase-change materials (PCMs) became popular due to their high optical contrast and non-volatility. PCMs have been employed as surrounding medium for plasmonic resonators and studies employing PCMs as all-dielectric metasurfaces are promising. The switching of PCMs by optical means lead to successful patterning in the µm-regime[2]. Bypassing the limits of diffraction imposed by optical switching, we employ a powerful thermal scanning probe lithography (t-SPL) technique to control position, depth and size of the switched PCM. First theoretical studies and metasurface designs for metasurfaces enabled by t-SPL could have exciting applications in the near infrared spectral range[3].

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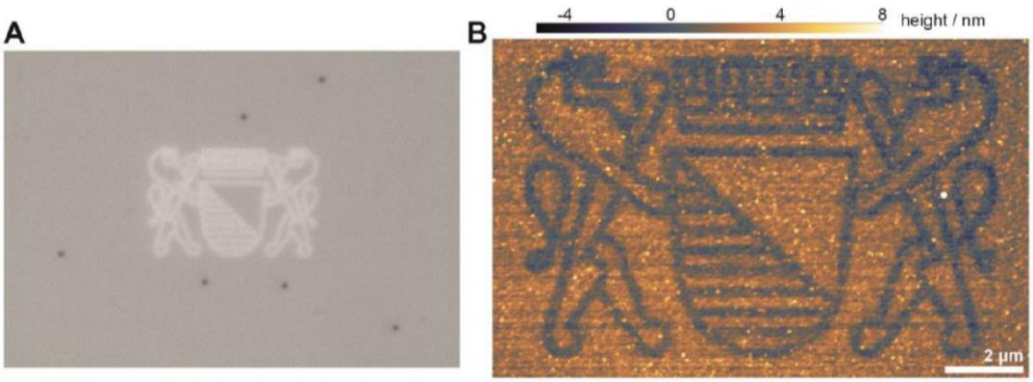

Tip-induced patterning of a 50 nm $Ge_2Te_3Sb_6$ thin film. (A) Optical micrograph of the amorphous film in between SiO_2 layers (5 nm above, 150nm below) on a Si substrate. (B) Topography image of the shown structure in A. The height decrease due to crystallization is observed. Feature sizes of down to 200nm can be patterned.

19 Guichard, Xavier

Interdependence of structural and compositional parameters on the luminescence of hafnia nanoparticles

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Luminescent materials are used in a variety of applications, from lighting and display technologies to scintillators for high-energy radiation detection.[1] A particular interest has grown towards nanoscale phosphors, proposed also for innovative bio-imaging excited by infrared radiation or photosensitizers for cancer self-lighting photodynamic therapy.[2]
The employment of nanoparticles in these applications relies on the ability to tailor their photo-physics, which is based on the control over structural features like their size, composition and crystal symmetry able to impact the photo-luminescence properties. Moreover, to be suitable for specific applications, the surface chemistry of these materials must be adapted to provide homogeneous stable dispersions/inks and thus facilitate handling and deposition, as well as efficient cell uptake.
Colloidal nanocrystals of HfO_2 can be synthesized from molecular precursors by a solvothermal route, where both fluorescence and structural control can be achieved thanks to the multifunctional role of rare earth (RE) doping.[3] While RE dopant ions activate the visible luminescence of nanocrystals, at the same time, their incorporation can also stabilise the cubic polymorph of HfO_2 at room temperature. Such a structural change can significantly affect the optical quality of sintered polycrystalline scintillator ceramics as well as the performance of RE-based upconversion. In addition, the native surface chemistry of such nanoparticles allows their further adaptation to either aqueous biological environments or, alternatively, to organic solvents.[4]
In this talk the control over the structure/function relationship in HfO_2 doped nanoparticles is discussed, together with its implications towards advanced bio-imaging and functional inks for innovative deposition/assembly of nanoparticle based optical materials.

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20 Ocana-Pujol, Jose

MoS_2 phase-change based thermo-chromic sensors

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MoS_2 is a van-der-Waals material that has attracted wide attention since the discovery that its electronic properties could be tuned with thickness[1]. The applicability of these properties remains undermined by the limitations of the techniques currently used to obtain thin-film MoS_2.
We have successfully fabricated 2D MoS_2 with thicknesses down to 2nm using magnetron sputtering, which, unlike other bottom-up technique commonly used to obtain MoS_2 like chemical vapor deposition, is known to produce large-scale thin films with uniform thicknesses[2]. Rutherford back scattering experiments show the substochiometric nature of this films, which could explain the anomalous electronic properties reported on magnetron sputtered MoS_2 on previous works[3].
X-Ray diffraction characterization confirms that the as-deposited films are amorphous and that they can be crystallized upon annealing. We show that the change in the optical properties of the material can be associated with its crystallization at temperatures starting at 300 degrees using ellipsometry and Raman spectroscopy.
This significant change (>10%) is more pronounced at the visible wavelengths, paving the way to the use of the material in temperature sensing applications. A proof of concept experiment demonstrated that using refractory metallic ZrO_xN_y as a substrate material.

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21 Kapsalidis, Filippos

Ultra-low Threshold Quantum Cascade Laser

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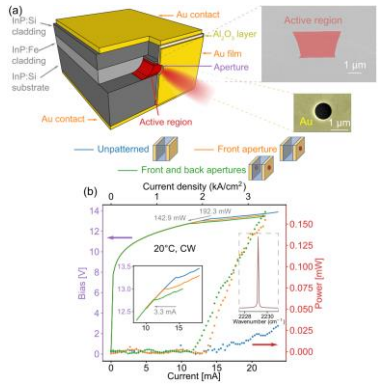
Quantum cascade lasers (QCLs) are widely used in the mid-infrared region for spectroscopic and gas-sensing applications. Due to the high operating voltage and typically Watt-level input power, bulky cooling systems are generally needed for driving a QCL at continuous-wave operation, which limit QCL applications on portable platforms. One approach for reducing the threshold dissipation power of a QCL is the combination of small volume devices, with state-of-the-art active regions and high reflectivity coatings on the facets. The reflectivity of the coatings is increased by patterning an aperture that generates a resonance, eventually enhancing reflectivity by 40%. The result is a device with, to our knowledge, record low lasing threshold and dissipation power (143 mW, 45% less than the previous record).



(a) Device geometry. (b) Device characterization.

22 Weigand, Helena

Metalenses from sol-gel based barium titanate for dynamic focus tuning

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Metasurfaces shape a new way of designing optical components that are much thinner than conventional ones. For instance, metalenses can focus a light beam by changing the electromagnetic wave front in the near field. This is achieved by an array of unit cells where the phase profile of the transmitted light is designed such that it interferes constructively in the focal point.[1] The spatial distribution of these cells depends on the intended polarization of light, its wavelength and the desired focal distance.

Apart from their scalability in fabrication, metalenses consist of much thinner materials than conventional bulk optics, enabling the possibility of dynamically tuning the lens' focal point. So far, this has been achieved by mechanically stretching the metalenses, orienting liquid crystals, or thermal heating of the material.[2] However, all of these processes operate on slow timescales and are difficult to integrate into everyday applications.
We present a strategy to rapidly modulate the focal point of metalenses using electric actuation of barium titanate. This optically nonlinear material is transparent in the visible range and exhibits a high electro-optic coefficient for changing its refractive index by applying a voltage.[3] We exploit these properties by fabricating a barium titanate metalens based on the Pancharatnam-Berry-Phase equation[4]. We use a highly scalable soft-nanoimprint process of barium titanate particles created via a sol-gel synthesis. We aim at dynamically tuning the focal distance of the metalens by the electro-optic effect of barium titanate. By this, fine-tuning of the focal distance in microscopy could be made easily accessible and color-resolving cameras could be replaced by simple photodiodes.

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23 Ritz, Christian

3D analysis of photoinduced forces by atomic force microscopy
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abstract confidential

Science & Technology of the Small

24 Stelmakh, Andriy

On the Mechanism of Alkylammonium Ligands Binding to the Surface of $CsPbBr_3$ Nanocrystals
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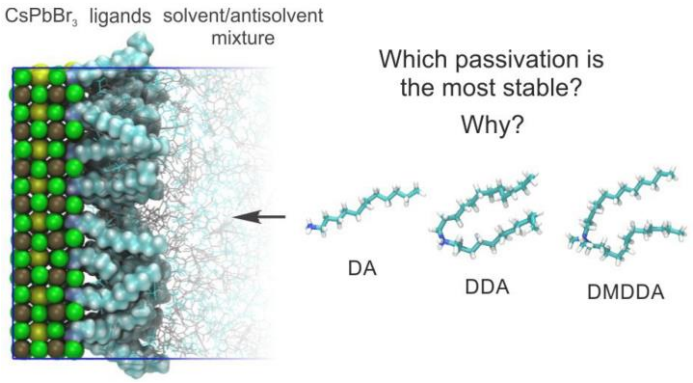
$CsPbBr_3$ nanocrystals suffer from instabilities caused by the dynamic and labile nature of both the inorganic core and the organic-inorganic interface. Surface ligand engineering therefore remains an imminent research topic. In this study, classical molecular dynamics simulations are used to gain insights into the inherent binding properties of three different alkylammonium ligands – primary dodecylammonium (DA), secondary didodecylammonium (DDA) and quaternary dimethyldidodecylammonium (DMDDA). Our simulations uncover three main factors that govern effective ligand–substrate interactions: (i) the ability of the head-group to penetrate into the binding pocket, (ii) the strength of head-group's interactions with the polar solvent, and (iii) higher barrier for ligand adsorption/desorption in the case of multiple alkyl chains. The interplay between these factors causes the following order of the binding free energies: DDA < DA = DMDDA, while surface capping with DDA and DMDDA ligands is additionally stabilized by the kinetic barrier. These findings are in agreement with experimental observations, wherein DDA is found to loosely bind to the CsPbBr3

surface, while DMDDA capping is more stable than capping with primary oleylammonium ligand. The presented mechanistic understanding of the ligand-nanocrystal interactions can be used to design new cationic ligands that make perovskite nanocrystal surfaces more robust.



25 Ussling, Frederic

Dynamics of homo- and heteronuclear clusters in intense X-ray pulses

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X-ray free-electron lasers (FELs) allow to image individual nanometer-sized biological specimen like viruses or large biomolecules with an unprecedented resolution using coherent diffractive imaging (CDI)[1]. The intense X-ray pulses, however, quickly destroy the object of interest, and the associated dynamics e.g. may blur the diffraction pattern and limit the resolution[2]. Thus, a profound investigation of intense X-ray matter interaction is inevitable for an unambiguous interpretation of the data. Clusters of atoms and molecules can serve as ideal model systems with the possibility to reduce the complexity to a degree where a link to theoretical modeling can be made. In an experimental study at the X-ray free-electron laser EuXFEL in Schenefeld, Germany, methane and neon clusters were irradiated with intense pulses at 1 keV photon energy and the resulting ionic fragments were measured. These systems are an ideal testbed to compare heteronuclear and homonuclear specimen. Both, neon and methane, are isoelectronic to each other (10 electrons in total) and have comparable masses. Furthermore, methane consists of carbon and hydrogen, emulating key aspects of biomolecules. We investigate the explosion dynamics of neon and methane clusters of different sizes and focal intensities. The ion spectra

of neon show high charge states up to Ne6+ with high kinetic energies. The ion spectra of methane clusters on the other hand are dominated by a strong proton signal with high kinetic energies up to 1 keV. The abundance of carbon is much lower and only singly charged carbon ions with low kinetic energies are observed. The observations indicate, that the fast ejection of the protons from the heteronuclear system efficiently “cools” the nanoplasma, which is further backed by theoretical modeling[3].

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26 Theiler, Pius M.

The gentle touch of mesoscopic Atomic Force Microscope tips
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abstract confidential

27 Saucedo-Espinosa, Mario A.

Electrochemical Synthesis of Gold Nanoparticles in Picoliter Droplet Reactors
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abstract confidential

28 Wohlwend, Jelena

Chemical Engineering of Quasi-perfect Absorption in Cu-Sn disordered network metamaterials
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abstract confidential

29 Tiwari, Preksha

Emission Control and Diameter Downscaling in InP Microdisk Cavities on Si by Au Incorporation
Preksha Tiwari, Anna Fischer, Pengyan Wen, Svenja Mauthe, Markus Scherrer, Noelia Vico Triviño, Marilyne Sousa, Daniele Caimi, Heinz Schmid and Kirsten E. Moselund
Materials Integration & Nanoscale Devices, IBM Research Zurich

Scaled cavities and emission control are important for efficient integrated photonics. Metals in nanolaser designs are used as a means to reduce the cavity dimension[1,2] and for enhanced modulation responses[3] due to their plasmonic nature and suitable thermal properties. Here we study heat sinking effects in Au-clad InP whispering gallery mode cavities (WGM) and show evidence of room-temperature lasing for 300 nm thick and 300 nm wide nanodisks, while the InP-only cavities lase only down to 500 nm.[4] Furthermore, we study the influence of Au nanoantennae on bonded InP microdisk cavities. Single mode emission is demonstrated by proper choice of antennae dimensions at room-temperature with stable emission down to 250 K. Identical WGM cavities without Au antenna are multimode and the dominant lasing mode changes upon temperature decrease. These results give insight into advantages of metals in nanolaser architectures and can potentially be extended to monolithically integrated devices as well. We thank the cleanroom operations team of the Binnig and Rohrer Nanotechnology Center (BRNC) for their help and support. This work was supported by the ERC StG PLASMIC (grant no. 678567).

[1] S. Wang et al., Nature Communications, 8(1), 2017.
[2] M. Aellen, et al., arXiv:2101.05881, 2021.
[3] C. Xu, et al., Optics Express 27(15), 2019.
[4] P. Tiwari et al., Optics Express 29(3), 2021.

Advanced Manufacturing

30 Binelli, Marco

Additive manufacturing of soft wearables with integrated sensors

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[1] Complex Materials, D-MATL, ETH Zurich
[2] Soft Transducers Laboratory, EPF Lausanne
[3] Cellulose and Wood Materials, Empa

abstract confidential

31 Das, Arnesh

Effect of Processing on the Air-void System of 3D Printed Concrete

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In the field of cement and concrete, many researchers have recently turned their focus towards the area of 3D printing. A number of research groups have already been able to achieve some degree of success. Most of these studies have focused on fresh material properties as the sole purpose has been to realize successful fabrication of structures. As a next step, it is equally important to ensure its proper long-term performance, from the point of view of both strength and durability. Freeze-thaw deterioration is one such durability issue, especially pertinent in cold places and it is likely to be more problematic for 3D printed structures due to the probable presence of cold joints. Air-entraining admixtures have been long added in concrete mixes to enhance its freeze-thaw protection but that has not necessarily meant that achieving robust and target air void systems has been easy. Changes in mix design and processing conditions can readily alter the void structure. In the present work, we study the effect of different

processing conditions involved in 3D printing. Some of these processes include pumping, acceleration/mixing and extrusion. The implications of these processes concerning frost damage are then assessed. A comparison of cast and printed samples after extrusion is also made.

32 Nydegger, Mirco

Electrohydrodynamic redox 3D printing: Towards multi-material additive manufacturing at the submicron scale

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[2] Department of Materials Science and Engineering, MIT

Small scale additive manufacturing (AM) provides unprecedented freedom in design in microscale engineering. When combined with the ability to control the chemical nature of each voxel deposited, small scale AM could unlock unique possibilities for tailoring mechanical, chemical, electrical, optical and magnetic properties of microstructures.
Yet, none of the micro- or nanoscale additive manufacturing processes can provide what microfabrication needs: the fast and reliable deposition of a wide range of device-grade materials, from insulators to semiconductors and metals, with a fast switching between different materials deposited[1]. Here, we will outline how electrohydrodynamic redox (EHD-RP) 3D printing can serve as a new toolbox to manufacture multi-material microelectronic devices[2]. The ink-free approach, based on the on-demand generation and reduction of metal ions, enables the local modification of the chemical composition in a voxel-by-voxel fashion. We will focus on the challenges involved in expanding the material's range of EHD-RP from Cu and Ag to a wide range of metals, semiconductors and insulators. The deposition of Zn structures and their subsequent thermal oxidation to semiconducting ZnO will be presented, together with an analysis of their structure and semiconductive properties. In addition, first steps towards the deposition of magnetic and insulating materials will be presented.

[1] L. Hirt, A. Reiser, R. Spolenak, T. Zambelli. Adv. Mater. 29, (2017).
[2] A. Reiser et al. Nat. Comm., 10, (2019).

33 Menétrey, Maxence

Electrohydrodynamic redox 3D printing: Achieving synthesis of microstructure gradients

Maxence Menétrey[1], Lukas Koch[1], Alain Reiser[1], Alla S. Sologubenko[2], Jeffrey M. Wheeler[1] and Ralph Spolenak[1]
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[2] Scientific Center for Optical and Electron Microscopy (ScopeM), ETH Zurich

While additive manufacturing (AM) at the macro-scale successfully made its way to industry and even individuals, its micro- and nano-scale counterpart would have the potential of revolutionizing microfabrication. Yet, combining high-resolution, geometry control, high-throughput together with device-grade synthesis of multi-materials still remains a challenge in the field[1].
Electrohydrodynamic redox 3D printing (EHD-RP) is an additive manufacturing technique with multi-metal capabilities and offering sub-micron spatial and chemical resolution in a single printing step[2]. In this work, we demonstrate the possibility of tuning materials properties in a voxel-by-voxel fashion. The applied voltage is shown to control not only the deposition rate but also the grain size and morphology of deposited copper pillars, thus opening the door for the synthesis of micro-devices with optimized

microstructure gradients. The material properties resulting from the different microstructure is further assessed by micro-compression experiments.

[1] A. Reiser, et al. Adv. Funct. Mater. 30, 1910491 (2020).
[2] A. Reiser, et al. Nat. Commun. 10, 1853 (2019).

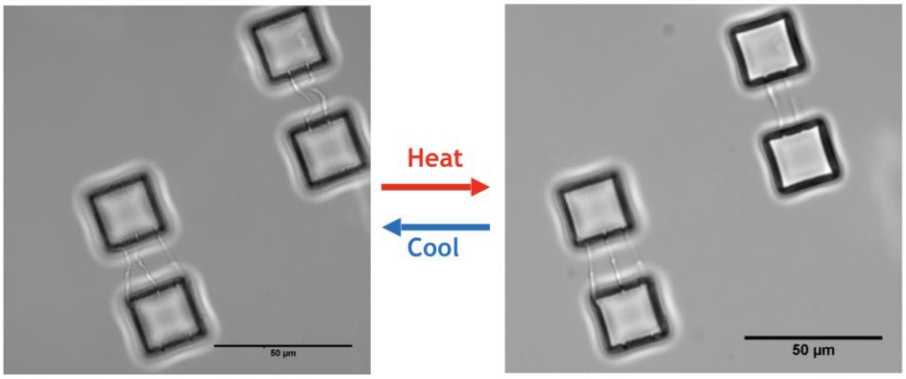
34 Shen, Xueting

Printing thermo-responsive sub-micron structures via Two-Photon Lithography

Xueting Shen, Steven van Kesteren and Lucio Isa
Soft Materials & Interfaces, D-MATL, ETH Zürich

Additive manufacturing has been intensively researched in the recent years, and special attention has been given to the fabrication of structures at the micro- and nanoscale. Two-photon lithography is a promising method used to fabricate and manipulate photosensitive hydrogels with nanoscale precision. In previous works, thermo-responsive structures in the 10 microns range have been successfully fabricated with two-photon lithography (TPL) using a pNIPAM-based photoresist. [1] However, these results can not be extended to fabrication at the sub-micron scale. With our work, we bring the scale of responsive structures printed with TPL down to the sub-micron range by optimizing compositions of the photo-resist. We further demonstrate the harvesting of these structures to obtain thermo-responsive Brownian objects of arbitrary shapes. Our results show potential for nanoscale fabrication of thermo-responsive materials and demonstrate the possibility to create complex temperature-controlled systems with shape reconfiguration. We anticipate the results of this project to have useful applications in micro-robotics, microfluidics and drug delivery.

[1] Marc Hippler, et. al. Nature Communications, 10(1):232, (2019).



Bright field image of single lines printed using the optimized PNIPAM resin between two PNIPAM blocks with a 100x oil immersion objective. The figure on the left shows the wiggly lines printed at room temperature. The figure on the right shows the straight lines heated above the transition temperature of PNIPAM.

35 Wagner, Marius

Fused Deposition Modelling of Stainless Steel Structures - from Binder Development to Sintered Properties

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[2] Laboratory for High Performance Ceramics, Empa

Additive manufacturing of metals by 3D printing of polymeric filaments containing high loadings of metal powder, subsequent debinding, and sintering offers a potent alternative to the widespread beam-based processes. The polymeric binder is the decisive component for a successful fabrication process. This study presents the development of a multi-component binder system for filament-based 3D printing of 316L stainless steel in various optimization steps. After printing, a two-step solvent – thermal debinding process is applied and finally the steel powder is sintered. 3D plate-lattices are fabricated and characterized to demonstrate the capabilities of the fused filament fabrication process using the developed filaments. The structures are able to undergo large plastic deformations without fracture and exhibit an extremely high energy absorption capability in compression testing.
The main contribution of this work is the development and disclosure of a binder system with two types of soluble polymers. This allows the precise control of the mechanical and rheological properties, as well as the backbone fraction of the binder. We envision this binder system as a platform which can be used for fabrication of various other materials. Based on the characterization experiments performed, it can be easily modified to adapt for other solid loadings, as parameters like stiffness, viscosity, or backbone content can be adjusted precisely.

36 Hille, Helge

Floating Isogeometric Analysis for Simulating Material Extrusion Processes

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[2] Department of Materials Science and Engineering, TU Delft

abstract confidential

37 Woigk, Wilhelm

Recycled carbon fibre into hierarchical natural fibre composites with high stiffness and damping

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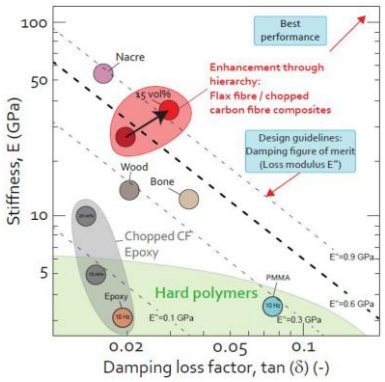
[1] Complex Materials, D-MATL, ETH Zurich
[2] Shaping Matter Lab, TU Delft

Continuous fibre-reinforced composites are lightweight and stiff, but show clear limitations in terms of vibration damping. Natural fibre composites have excellent damping characteristics and can be produced at much lower environmental cost, yet their properties cannot rival those of their synthetic counterparts, limiting their design freedom. In this study, we additively combine natural and recycled carbon fibres into multi-directional composites to overcome design constraints, to increase the component's stiffness and vibration damping behaviour and to enhance the sustainability of lightweight parts.



Comparison of in-plane stiffness and damping loss factor

38 Volk, Maximilian

Thermal management of thermoplastic composite pultrusion for large cross-section profiles

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[1] Composite Materials & Adaptive Structures, D-MAVT, ETH Zurich
[2] Schulich School of Engineering, University of Calgary

Pultrusion is a rapid and cost-effective manufacturing technology for continuous fibre reinforced thermoplastic composite profiles. As the cross-sections of pultruded profiles grow to meet increasing performance requirements, manufacturing challenges concerning heat transfer are encountered, that are investigated in this study. A two dimensional finite element model was used to simulate the heat transfer and fluid flow physics of the pultrusion process for increasing diameters from Ø5- Ø40 mm. To facilitate the experimental validation, a novel batch-wise pultrusion concept, represented through Fig. 9 is introduced in which the impregnation process is observed in-situ using a transparent die. The pultrusion studies using a tailor-made manufacturing set-up depicted in Fig. 10 (a) with amorphous polyethylene terephthalate/glass fibre (PET-GF) commingled yarns show that with proper design, pultrusion is able to deliver consistent, high quality (void content < 2%) profiles up to at least Ø 40 mm as shown in Figure 10 b.

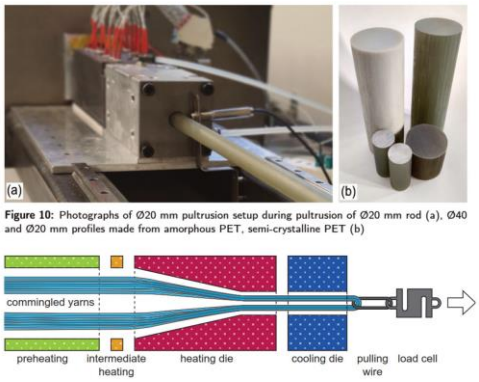

Figure 10: Photographs of Ø20 mm pultrusion setup during pultrusion of Ø20 mm rod (a), Ø40 and Ø20 mm profiles made from amorphous PET, semi-crystalline PET (b)

Pultrusion process for sample manufacturing.

39 Zhang Zhiyuan

Microswarms Rolling in Acoustic Virtual Walls

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Micro- and nanorobotics could become a powerful tool that would allow specialized tasks in medicine, including non-invasive surgical procedures and drug delivery to hard-to-reach sites. However, manipulation at the microscale is challenging, typically requiring a nonreciprocal movement of the robot to propel. An alternate and widely used manipulation strategy is rolling; however, the concept is restricted to the walls or boundary conditions. Here, we demonstrate microswarms rolling in mid-liquid for the first time in the absence of any walls by combining acoustic and magnetic fields. Pressure nodes of the acoustic standing wave field mimic the virtual walls. The rotating magnetic field was employed to self-assemble and rotate the superparamagnetic microswarms. By switching the acoustic virtual wall pattern and the magnetic field rotational direction, we achieved the microswarm manipulation in arbitrary acoustic virtual walls to draw the "E", "T", and "H" letters, without the limitation of any surface or boundary conditions. The newly presented microswarm manipulation strategy will provide an exciting transport and delivery technique to science and engineering disciplines.

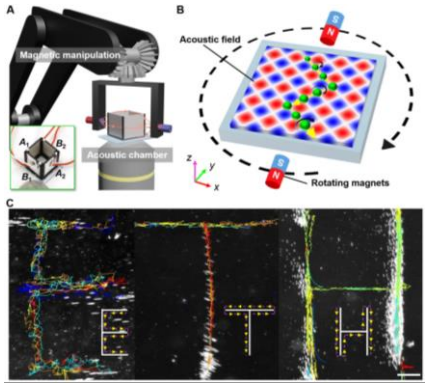

Illustration of microswarms rolling in acoustic virtual walls. (A) The experimental setup consists of the magnetic effector held and rotated by the robotic arm and the acoustic chamber mounted on the inverted microscope. The insert shows details of the acoustic chamber. (B) Microswarms exhibit rolling-like motion in the combined two-dimensional acoustic standing wave field and the rotating magnetic field. (C) Microswarms write the word "ETH" by the tracked trajectory. Scale bar, 100 µm.

40 Bailey, Maximilian

Janus Nanoparticle Deposition: A Versatile Platform Towards A Microswimmer-Based Reactor

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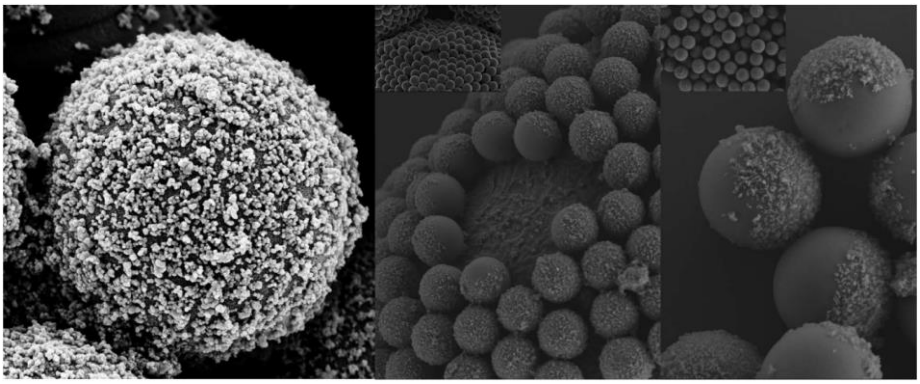
[1] Soft Materials & Interfaces, D-MATL, ETH Zurich
[2] Surface Science & Technology, D-MATL, ETH Zurich

The application of nanoparticles to heterogeneous photocatalysis has been the subject of extensive research due to their promising activity and versatility. Nevertheless, these nano-catalysts suffer from the same mass and light transfer limitations as other conventional heterogeneous photocatalysts, as well as the additional challenges faced when supporting the nanoparticles on more processable materials. We draw upon the seemingly unrelated research field of active matter to develop a strategy which might help address the dual issues of nano-catalyst support and mass transfer limitations. Specifically, micron-sized 'Janus' active colloids asymmetrically decorated with photocatalytic nanoparticles have been produced via a Pickering wax emulsion-based fabrication technique.

Supporting the nanoparticle photocatalysts onto microparticles significantly enhances their processability, enabling separation techniques such as simple gravitational filtration or centrifugation. More importantly, we propose that the autonomous motion of the active colloids can improve overall catalytic rates. We hypothesise that the movement of the active colloids sets the surrounding fluid into motion, in turn enhancing localised mass transport. We thus aim to demonstrate an increase of reaction rates by utilising a mobile catalyst platform, with the long-term objective of designing a photocatalytic reactor concept employing particles with a dual catalyst-stirrer functionality.



Overview of the fabrication process. Left: Nanoparticle attachment to SiO_2 microparticles. Centre: Asymmetric functionalisation of SiO_2 microparticles using the Pickering wax emulsion technique. Right: Janus Microswimmers.

41 Del Campo Fonseca, Alexia

Acoustic microswarm robotics in artifitial vasculatures
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Acoustic Robotics for Life Science & Healthcare, D-MAVT, ETH Zurich

abstract confidential

42 Dillinger, Cornel

Starfish-inspired Ultrasound-driven Soft Microrobot
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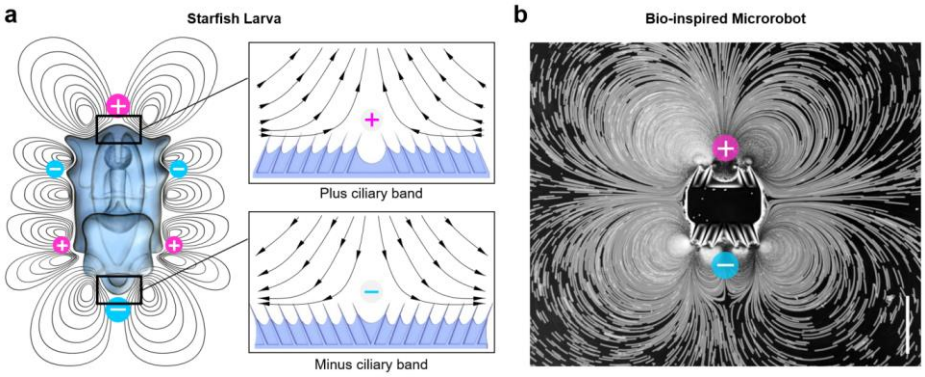
[1] Acoustic Robotics for Life Science & Healthcare, D-MAVT, ETH Zurich
[2] Department of Surgery, University of Michigan

In this project, we present the first demonstration of ultrasound-activated synthetic ciliary bands, inspired by the natural arrangements of cilia on the surface of starfish larva. Our polymeric ciliary bands are exposed to a high-frequency acoustic field, which forces the cilia into small-amplitude oscillations [1]. The vicinity of cleverly arranged oscillating ciliary arrays generates controllable steady-state bulk streaming. When planar ciliary arrays are angled toward each other (/// \\\), named as a “+” ciliary band arrangement, the fluid is pushed away from the surface on which the cilia are arranged (analogous a source). In contrast in a “–” ciliary band arrangement, cilia are angled away from each other (\\\ ///) and the liquid is forced in toward the band (analogous a sink). We incorporated these findings to develop a new physical principle for acoustic-based propulsion at the microscale. The propulsion mechanism is based on high-frequency small-amplitude oscillations of ciliary bands that locally introduce considerable inertial forces. We further demonstrate the functional diversity of synthetic cilia. By placing + and – ciliary

bands adjacent to each other, we developed a microparticle trap analogous to the feeding mechanism of starfish larvae.

[1] N. Nama, et al., Lab on a Chip 14.15 (2014).



Starfish larva-inspired ultrasound ciliary band designs. (a) A starfish larva exhibits a complex flow profile of counter-rotating vortices generated by series of + and – ciliary bands arranged on its body protuberances. (b) A starfish-inspired microrobot consisting of a + (top) and a – (bottom) ciliary band placed in a tracer solution. The ciliary bands oscillate when actuated by ultrasound, producing complex flow profiles similar to those observed with its biological counterpart. Scale bar, 250 µm.

43 Durrer, Jan

A Multifunctional Acoustofluidic End Effector for Microscale Liquid Manipulation

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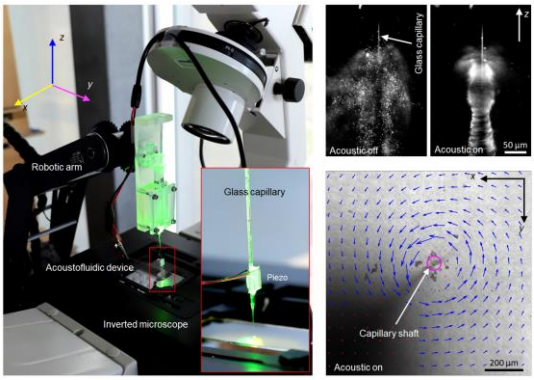
[2] Department of Surgery, University of Michigan
[3] Department of Molecular Life Sciences, University of Zurich

Liquid manipulation is the foundation of most laboratory processes. For macroscale liquid handling, many robotic systems require large quantities of expensive reagents, and most lack support for sample preparation at the microscale. Lab-on-a-chip systems have come to serve for microscale liquid manipulation; however, the technology is lacking in automation and multifunctionality. Despite the potential synergy between robotics and microfluidic systems, no suitable interface exists to link both fields of research yet. We present a robot-assisted acoustofluidic manipulation system, comprising a robotic arm and an acoustofluidic end effector, that combines macroscale robotics and microfluidic functionalities. The new capillary-based acoustofluidic device yields a steady-vortex, corkscrew-like flow around the capillary towards the capillary tip. To demonstrate its unprecedented versatility and multifunctionality, we carried out pumping, droplet merging, and mobile mixing of complex viscous liquids, all without the need for additional Lab-on-a-chip devices. Fig. 1 depicts the experimental setup, and the circular flow induced into the surrounding liquid by the capillary once it is excited using ultrasound. Finally, we preprogrammed our system to perform automated mixing of viscous liquids in well plates, illustrating its versatility for the automatic execution of chemical processes.



Experimental setup and working principle of the acoustofluidic device.

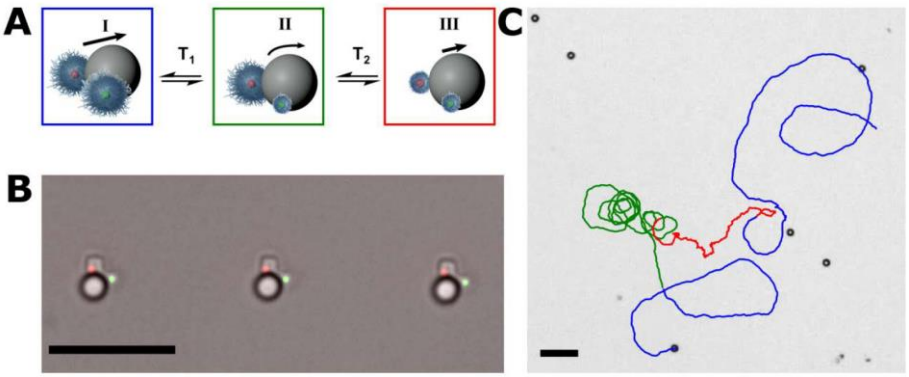
44 Van Kesteren, Steven

Responsive colloidal molecules as internally-controlled microswimmers with multi-state dynamics

Steven van Kesteren, Laura Alvarez and Lucio Isa
Soft Materials & Interfaces, D-MATL, ETH Zurich

Active colloids are seelf-propelled micro-scale objects that serve as model systems for biological microscopic swimmers. The ability of microswimmers to autonomously sense and adapt to their environment is widespread throughout nature, and synthetic analogues are key in the development of micro-scale robotics. However, synthetic microswimmers lack any autonomous self-regulation and typically rely on external feedback schemes to control their motion. Here, we show the fabrication of colloidal molecules with soft and hard components, which serve as internally controlled microswimmers propelled by induced-charge electrophoresis. These colloidal molecules are purpose-built clusters of PNIPAM-co-AAC thermoresponsive microgels using sequential capillary assembly[1] which allows an unprecedented control over the geometry and composition. Clusters with multiple microgels exhibit multi-state motilities controlled by temperature. We rationalize the different motilities of these states by temperature-induced changes in shape and dielectric properties[2]. Hereby, we demonstrate a rich class of responsive microswimmers with properties akin to simple soft robots. In the future, additional components in our synthetic microswimmers could provide them with different responses and inter-particle communication schemes to potentially reach “nature-like” sensing and collective motion.

[1] Ni, S., Leemann, J., Buttinoni, I., Isa, L. & Wolf, H. Sci. Adv. 2, (2016).
[2] Alvarez, L. et al. Submitted (2020).



(A) Schematic of a multi-state responsive microswimmer. (B) Composite brightfield-fluorescence micrograph of colloidal molecules C. Example trajectory of a microswimmer switching between state I (blue), state II (green), state III (red). (scale bars are 10 μm)

Strength & Durability of Materials

45 Aguzzi, Giulia & Zaccherini Rachele

Lattice Metastructures for Elastic Wave Control

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Structural Mechanics & Monitoring, D-BAUG, ETH Zurich

Lattice metastructures, periodic arrangements of engineered unit cells, have proven capable of controlling wave propagation across different wavelength scales. This stems from the presence of bandgaps in the band diagram, which designate frequency ranges where the wave propagation is arrested. These originate from local resonance or Bragg scattering interference. Recent works have shown that such a bandwidth can be enlarged by incorporating inertial amplification mechanisms within the lattice unit cell.
Here, we report two classes of metastructures. First, we examine the well-known octet lattice[1], whose cellular architecture stems from the interweaving of twelve beams. While in the long wavelength limit, the periodic tessellation of this cell resembles an equivalent homogeneous material featuring anisotropically propagating waves, at higher frequencies its behavior is far from being obvious. Short elastic waves interact with the detailed network of the cell and are retained by the bending local resonance of the constituent struts. This behavior, typically unexpected in a single block material, reveals the potential of this structure in wave control applications as well as the flexibility of its design parameters.
In the second metastructure, we employ opposite-chiral connections to couple the axial and rotational motion of the mass elements, thus amplifying the inertia of the system[2]. In particular, the building block consists of a hollow-square plate connected to a ring through four arch-like ligaments. Simplified analytical and finite element models of the representative unit cell are developed to obtain the dispersion properties of the infinite diatomic lattice. A wide stop band is found, with a bandwidth, which considerably exceeds the one achieved by means of conventional band gap generation methods.

[1] G. Aguzzi, et. al., Proc. of ISMA, pp. 2545-2554 (2020).
[2] R. Zaccherini, et. al., Proc. of ISMA, pp. 2563-2574 (2020).

46 Schmid, Thilo

Discretizing Pore Structure at the Steel-Concrete Interface for Transport Modeling

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[1] *Durability of Engineering Materials*, D-BAUG, ETH Zurich
[2] Oregon State University, USA

Investigations of reinforcement corrosion in concrete rely on reactive transport modeling to describe the relevant underlying physical and chemical processes. Traditional models employ some form of homogenization of different transport mechanisms of species in a representative volume element, thus generating macroscopically relevant quantities that are measurable by practical experiments. Such parameters include bulk porosity, formation factor, and effective ionic diffusion coefficients. This simplification also has the benefit of allowing large-scale simulations with limited computational

resources. Despite its practical advantages, the homogenization approach does not explicitly consider the heterogeneous nature of the porous medium, especially at the steel-concrete interface, where the microstructure is complex and significantly different from that of bulk concrete[1]. Furthermore, this zone is subject to extreme concentration and electrical potential gradients due to the electrochemical reactions that take place on the steel surface. Therefore, for fundamentally understanding and predicting reinforcement corrosion, there is need for accurate modeling of reactive transport processes in the steel-concrete interface. However, the first step for such modeling efforts is the establishment of a realistic discretized domain that can capture the heterogeneous nature of the steel-concrete interface.
This study explores a novel approach of obtaining a three-dimensional discretized domain (to be used by reactive transport models) directly from a real concrete sample using SEM imaging of successive surfaces prepared by focused ion beam (FIB) micro-milling. Upon segmentation into the different constituent phases, the three-dimensional data are turned into a multi-part finite element mesh. A discretized domain obtained in this way eliminates the need for property and geometry homogenization, and allows for a more realistic modeling of moisture and ionic transport in the pore network using the explicit relevant transport mechanisms.

[1] U. Angst, et al., Mater Struct 50, 143 (2017).

47 Albertini, Gabriele

Dynamic Fracture of Heterogeneous Materials
Gabriele Albertini[1,2], Mathias Lebihain[3], François Hild[4], Laurent Ponson[3] and David S. Kammer[1]
[1] Computational Mechanics of Building Materials, D-BAUG, ETH Zurich
[2] School of Civil and Environmental Engineering, Cornell University
[3] Institut Jean le Rond d'Alembert, Sorbonne Université
[4] Laboratoire de Mécanique et Technologie (LMT), ENS Paris-Saclay

We investigate dynamic fracture of heterogeneous materials by measuring near crack-tip displacement fields as the rupture propagates through a periodic array of obstacles of contrasting toughness. We provide direct evidence of crack speed jumps at the boundary of obstacles. Our experiments reveal that such a discontinuous dynamics emerges from the combination of rate-dependent fracture energy and inertia, which allows the crack to cross a fracture energy discontinuity at constant energy release rate. We show that the Linear Elastic Fracture Mechanics (LEFM) equation of motion for a crack is applicable for cases with strong variation of fracture energy. The rate-dependency is a direct consequence of the out-of-equilibrium nature of the fracture phenomenon and is often neglected. However, it plays a central role in setting up homogenized toughness.

Electromagnetic Materials & Processes

48 Liu, Zhentao

Chiral coupling-induced asymmetric domain wall motion
Zhentao Liu[1], Zhaochu Luo[1], Stanislas Rohart[2], Laura J. Heyderman[1], Pietro Gambardella[3] and Aleš Hrabec[1,3]
[1] Mesoscopic System, D-MATL, ETH Zurich and PSI
[2] Laboratoire de Physique des Solides, Universite Paris-Saclay
[3] Magnetism & Interface Physics, D-MATL, ETH Zurich

The engineering of chiral coupling in thin magnetic films with inhomogeneous anisotropy[1] allows for designing synthetic magnetic systems of fundamental and technological interest[2,3]. This coupling arises from the interfacial Dzyaloshinskii-Moriya interaction, which, in combination with spin-orbit torques, leads to the local manipulation of chiral magnetic order[4]. So far, the chiral coupling between nanomagnets with patterned magnetic anisotropy has been studied only in Pt/Co/AlOx trilayers.
Here we design a system for quantifying the chiral coupling based on field- and current-induced asymmetric domain wall motion in Pt/Co/AlOx racetracks. This establishes a versatile method to characterize the chiral coupling in different materials. We further provide evidence of chiral coupling in Pt/CoB/AlOx trilayers with ultralow pinning. We show that the domain walls in such a system propagate in response to the DMI effective field even in the absence of any external driving force. This work shows that the chiral coupling can be used to locally design intrinsic fields that affect the magnetization dynamics.

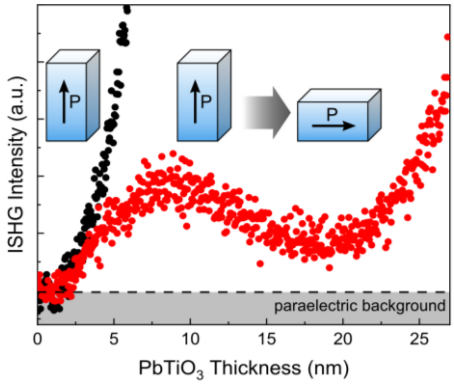
[1] Luo et al. Science 363, 1435 (2019).
[2] Luo et al. Nature 579, 214 (2020).
[3] Dao et al. Nano Lett. 19, 5930 (2019).
[4] Hrabec et al. Appl. Phys. Lett. 117, 130503 (2020).

49 Sarott, Martin

Tracking ferroelectric domain formation during epitaxial thin-film growth
Martin F. Sarott, Manfred Fiebig and Morgan Trassin
Multifunctional Ferroic Materials, D-MATL, ETH Zurich

Ferroelectric materials with a switchable spontaneous polarization are promising candidates for the design of energy-efficient next-generation devices in oxide electronics. A crucial hurdle in this endeavor is the difficulty in controlling the polarization state, i.e. the arrangement of domains and domain walls that constitute the functional entities of ferroelectrics. Achieving this control is of particular importance in the technologically relevant ultrathin regime. Here, we overcome this notorious difficulty by tracking in-situ, during growth, the formation of ferroelectric domains in epitaxial films of the ferroelectric model system PbTiO3. By combining in-situ optical second harmonic generation (ISHG) with post-growth piezoresponse force microscopy and SHG imaging, we identify the emergence of a ferroelectric polarization and the thickness threshold at which domain formation spontaneously occurs[1]. Furthermore, by tailoring the epitaxial strain, we establish a way to act on this domain formation and achieve deterministic domain configurations in thin films.
Thus, our in-situ approach provides us with an unprecedented direct access to the epitaxial strain dependent ferroelectric domain nucleation, which is key for the design of thin films with predefined domain states for reliable ferroelectric properties in the ultrathin regime.

[1] M.F. Sarott, et. al., Appl. Phys. Lett. 117 132901 (2020).



Out-of-plane polarization signature during the growth of $PbTiO_3$ without (black) and with (red) the exertion of tensile epitaxial strain.

50 Tosic, Tara

Coupling between structure and magnetism in the hexagonal manganites

Tara Tosic[1], Nicola Spaldin[1] and Quintin Meier[2]
[1] Materials Theory, D-MATL, ETH Zurich
[2] LITEN, CEA Grenoble

We use density functional calculations and structural analysis to determine how the charge redistribution associated with specific structural distortions plays a crucial role in determining the magnetic order in the multiferroic hexagonal manganites. Understanding the detailed relationship between magnetic ordering and crystal structure in multiferroic materials is a crucial step in engineering novel, technologically relevant properties for applications such as magnetocalorics or memory devices. Using hexagonal yttrium manganite, h-$YMnO_3$, as our prototype we show that the so-called K1 distortion mode, corresponding to an (ab) planar displacement of the Mn and apical Oxygen ions, plays a key role in determining the magnetic order of the system. We derive a K1-mode dependent magnetic Hamiltonian which correctly predicts the experimentally measured magnetic ground state of h-$YMnO_3$ at 6K [1]. We calculate how the magnetic order evolves with the size of the K1 distortion, and show that our magneto-structural coupling model can be generalized to the whole series of materials in this family of crystals.

[1] S. Lee et al., Nature Lett. (2008).

51 Mansouri Tehrani, Aria

Machine learning exploration of ferroelectric materials

Ramon Frey, Aria Mansouri Tehrani, Bastien Grosso and Nicola Spladin
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We report the development of a combined machine learning and high-throughput DFT framework to accelerate the search for novel ferroelectrics. This framework is capable of predicting potential ferroelectric compounds using only compositions as input. Initially, for a given composition-space, a series of machine learning algorithms predict the possible stable stoichiometries that are insulating and have a non-centrosymmetric structure, necessary for the ferroelectricity. A final classification model then predicts the point groups of these stoichiometries. Based on the point groups, a subsequent series of high-throughput DFT calculations determine the ground state crystal structure. As a final step, using group theory considerations, non-polar parent structures are identified and the polarisation values are further determined. By predicting the crystal structures as well as the polarisation values, this method provides a powerful tool to explore new ferroelectric materials beyond the existing databases.

52 Aeschlimann, Jan

Multiscale Modeling of Conductive Bridging Random Access Memories: from Ab Initio to Finite Elements

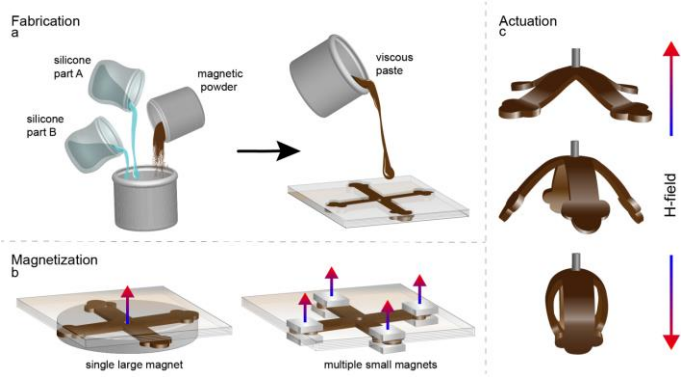
Jan Aeschlimann, Christoph Weilenmann, Fabian Ducry, Alexandros Emboras and Mathieu Luisier
Integrated Systems Laboratory, D-ITET, ETH Zurich

53 Carpenter, Julia

Facile Manufacturing Route for Magneto-Responsive Soft Actuators

Julia A. Carpenter[1], Thomas B. Eberle[1], Simone Schürle[2], Ahmad Rafsanjani[1,3] and André R. Studart[1]
[1] Complex Materials, D-MATL, ETH Zurich
[2] Responsive Biomedical Systems, D-HEST, ETH Zurich
[3] current: Center for Soft Robotics, University of South Denmark

Magnetically driven soft actuators are unique because they are fast, remote-controlled, conformal to rigid objects, and safe to interact with humans. Despite these multiple functionalities, a broader utilization of such actuators has been hindered by the high cost and equipment-intensive nature of currently available manufacturing processes. Here, we describe a simple fabrication route for magneto-responsive soft actuators using cost-effective and broadly available raw materials and equipment. The method utilizes castable silicone resins that are loaded with magnetic particles and subsequently magnetized under an external magnetic field. The experimental investigation of silicone-based composites prepared with particles of distinct chemistries, sizes, and morphologies enabled the identification of the raw materials and magnetization conditions required for the process. This led to functional soft actuators with programmable magnetic patterns that are capable of performing pick-and-place, lifting, catching, and moving tasks under the remote action of an external magnetic field. By removing manufacturing hurdles associated with costly raw materials and equipment, we expect the proposed approach to facilitate the design, implementation, and exploitation of the unique functionalities of magneto-controlled soft actuators in a wider number of applications.



Scheme illustrating the (a) fabrication, (b) magnetization, and (c) actuation of silicone parts loaded with magnetic particles.

54 Mattich, Iacopo

Color Formation From the Assembly of Superparamagnetic Colloidal Assembly Under Time-Varying Magnetic Fields

Iacopo T. Mattich[1], Golnaz Isopour[2], Ahmet Demirörs[1], Simone Schürle[3], Marco Lattuada [4] and André R. Studart[1]
[1] Complex Materials, D-MATL, ETH Zurich
[2] Department of Mechanical Engineering, MIT

[3] Responsive Biomedical Systems, D-HEST, ETH Zurich
[4] Department of Chemistry, University Fribourg

abstract confidential

55 Pac, Aleksandra

Unconventional computing with ferromagnetic heterostructures

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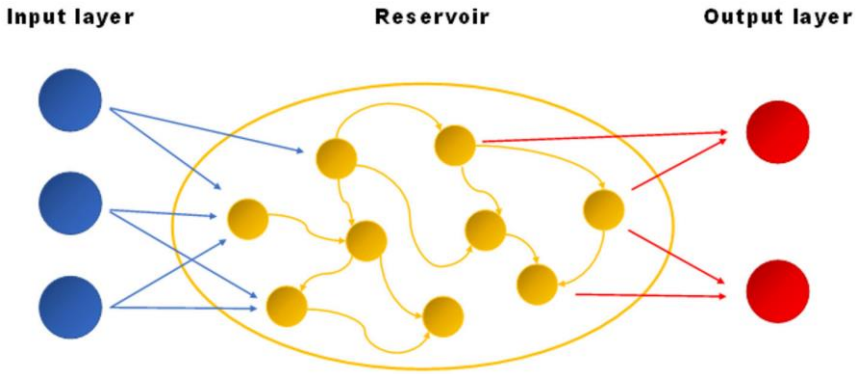
[1] Mesoscopic System, D-MATL, ETH Zurich and PSI
[2] Magnetism & Interface Physics, D-MATL, ETH Zurich

The need for increased computational capabilities for the next generation of devices poses a significant challenge for the future, with the focus being on the reduction of power required for data processing in a society moving towards full automation. One solution is to look for alternatives to the conventional von Neumann framework, where the von Neumann bottleneck is replaced with architectures inspired by biological processes, allowing for parallel computation[1].
Here we investigate computation using ferromagnetic heterostructures, where the dynamics between different nodes can resemble that of artificial neural networks[2]. We are exploring possibilities for control of our structures using spin-orbit torques[3], with the end goal aiming for full electrical control of the system. We will focus on implementing them into systems such as logic gates and reservoir computing[4], which will eventually allow for pattern classification.

[1] J. Grollier, D. Querlioz & M.D. Stiles, Proc. IEEE (2016).
[2] J.J. Hopfield, Proc. Nat. Acad. Sci. (1982).
[3] J. A. Nance at al, IEEE Trans. Mag. (2020).
[4] G. Tanaka et al, Neural Netw. (2019).



A typical reservoir computing framework, where in this case the reservoir is replaced with an array of ferromagnetic dots that interact via dipolar coupling. The only training required is between the reservoir and the output layer, while the nodes within the reservoir remain fixed.

56 Verbeek, Xanthe H.

Hidden Magnetoelectric multipoles, and anti-magnetoelectric effect in Fe_2O_3

Xanthe H.Verbeek and Nicola A.Spaldin
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We present first-principles calculations of the magnetoelectric multipoles in Cr_2O_3 and its iron-based analogue, Fe_2O_3. Cr_2O_3 is the prototypical linear magnetoelectric material, in which an applied magnetic field induces a proportional electric polarization and vice versa, a process which can be understand in terms of the ferroic ordering of magnetoelectric multipoles[1]. Fe_2O_3 has the same structure as Cr_2O_3 but a different magnetic ordering which does not allow a linear magnetoelectric response. We used a group theory analysis to determine the allowed magneteelectric moments on the transition metal and oxygen ions in both materials. We complement this with a density functional theory calculation with the LDA+U method in an extension[2] to the VASP code[3]. In Cr_2O_3 we find local magnetoelectric monopoles and quadrupoles consistent with the established magnetoelectric effect. Surprisingly, our calculations revealed hidden magnetoelectric multipoles on the iron ions in Fe_2O_3, with the multipoles on adjacent ions having opposite sign consistent with the absence of a net magnetoelectric effect. We predict an anti-magnetoelectric effect in Fe_2O_3, in which pairs of spins cant in opposite directions under the application of an external electric field, to create an additional anti-ferromagnetic ordering along the axis of the applied field. We discuss possible consequences of this effect for bulk Fe_2O_3 and heterostructures of Fe_2O_3 and Cr_2O_3.

[1] N. A. Spaldin et al., J. Phys.: Condens. Matter, 20, 434203 (2008).
[2] F. Thöle and N. A. Spaldin, Phil. Trans. R. Soc. A, 376, 20170450 (2018).
[3] G. Kresse, J. Furthmüller, Phys. Rev. B, 54, 1169 (1996).

57 Matas, Marek

Density functional theory searches for next generation materials of dark matter detection experiments

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We use density functional theory combined with quantum field theory to calculate the signal from light dark matter interacting with the electrons in conventional materials.
The visible matter contributes a small fraction of the total mass of the universe that we currently observe. The majority of this mass is thought to be hidden in the form of an unidentified particle, the so-called dark matter (DM), and its direct detection has proven to be one of the most challenging scientific projects of today. It is becoming increasingly difficult to build a detector that would be sensitive to low energy depositions expected from DM while still maintaining a relatively background-free signal. We have used the techniques of density functional theory to model materials currently used in these experiments in order to predict a signal that would be observed once DM is detected. We calculate the wavefunction of the electrons bound within various crystals and connect it with the scattering probabilities coming from dark matter models within quantum field theory. We then produce signal rate and intensity depending on the considered dark-matter-particle which would help us to identify its intrinsic properties. We have used this formalism to put constraints on the current experiments using silicon and germanium targets as well as working on extending it to include materials of the future-planned detectors.

"We have enjoyed the organisation of this year's MaP Graduate Symposium and hope that you will have a good experience throughout the two days. If you are interested in joining next year's organising committee, feel invited to contact Larissa Schefer."

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