



WESTFÄLISCHE
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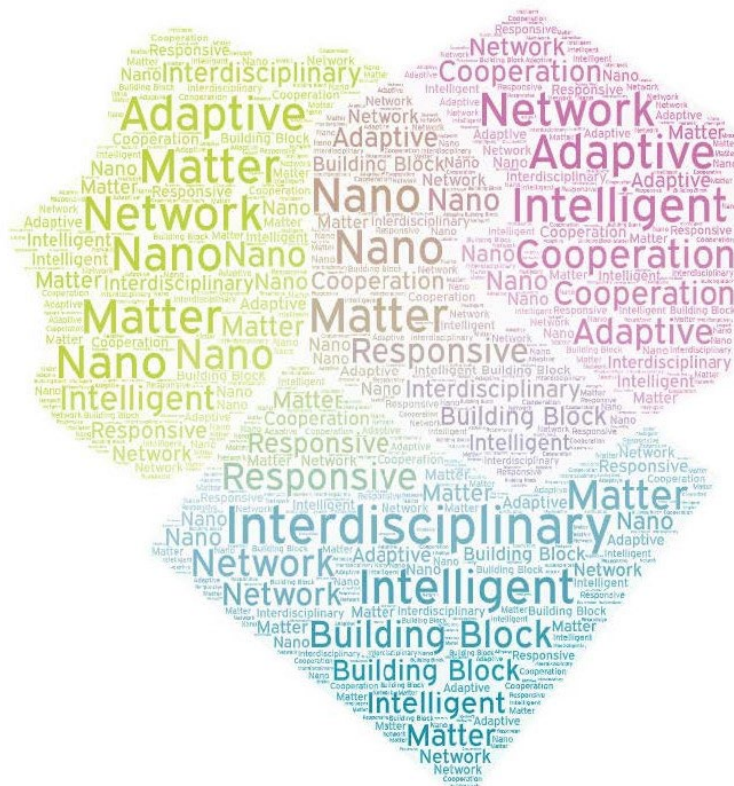
Center for Soft Nanoscience



INTELLIGENT
MATTER

2nd Münster Symposium on Intelligent Matter

June 14th, 2023
Münster, Germany



Book of Abstracts

MüSIM2023 Speakers



Prof. Dr. Marjolein Dijkstra

Utrecht University

Debye Institute for Nanomaterials Science

Soft Condensed Matter

Utrecht, The Netherlands

Marjolein Dijkstra is full professor (2007) in the Debye Institute for Nanomaterials Science at Utrecht University. She received an MSc degree in Molecular Sciences at Wageningen University as well as an MSc degree in physics at Utrecht University. She obtained her PhD degree from Utrecht University in 1994 under the supervision of Daan Frenkel, and was awarded twice a prestigious EU Marie Curie Individual Fellowship to join the Physical and Theoretical Chemistry group at Oxford University and the H.H. Wills Physics Laboratory at Bristol University. She was a research associate at Shell Research in Amsterdam in 1995. In 1999, she started her own research group at Utrecht University, focused on obtaining fundamental understanding on the self-assembly behavior of soft materials, and how the self-assembly process can be manipulated by external fields such as gravity, templates, air-liquid or liquid-liquid interfaces, and electric fields. Her group employs theory, computer simulations, and machine learning to study physical phenomena in soft-matter systems like self-assembly in colloidal dispersions (crystals, quasicrystals, and exotic liquid crystals of odd-shaped particles), glass and jamming transitions, active matter, crystal nucleation, and inverse design of new soft materials. She is recipient of the Minerva Prize (2000), a high-potential grant (2004), a prestigious NWO VICI and Aspasia grant (2006), and an ERC advanced grant (2020), and is elected as member of the Royal Netherlands Academy of Arts and Sciences (KNAW) in 2020.

Machine Learning and Inverse Design of Soft Materials

Marjolein Dijkstra, Utrecht University, The Netherlands

Predicting the emergent properties of a material from a microscopic description is a scientific challenge. Machine learning and reverse-engineering have opened new paradigms in the understanding and design of materials. However, this approach for the design of soft materials is highly non-trivial. The main difficulty stems from the importance of entropy, the ubiquity of multi-scale and many-body interactions, and the prevalence of non-equilibrium and active matter systems. The abundance of exotic soft-matter phases with (partial) orientation and positional order like liquid crystals, quasicrystals, plastic crystals, along with the omnipresent thermal noise, makes the classification of these states of matter using ML tools highly non-trivial. In this talk, I will address questions like: Can we use machine learning to autonomously identify local structures, detect phase transitions, classify phases and find the corresponding order parameters, can we identify the kinetic pathways for phase transformations, and can we use machine learning to coarse-grain our models? Finally, I will show in this lecture how one can use machine learning to reverse-engineer the particle interactions to stabilize nature's impossible phase of matter, namely quasicrystals?

MüSIM2023 Speakers



Prof. Dr. Peer Fischer

Heidelberg University

Institute for Molecular Systems Engineering and
Advanced Materials

Heidelberg, Germany

Peer Fischer is a Professor of Experimental Physics (Molecular Systems Engineering) and he heads the independent Micro Nano and Molecular Systems Lab at the Max Planck Institute for Medical Research in Heidelberg.

Peer Fischer received a BSc. degree in Physics from Imperial College London and a Ph.D. from the University of Cambridge. He was a NATO (DAAD) Postdoctoral Fellow at Cornell University, before joining the Rowland Institute at Harvard. At Harvard he held a Rowland Fellowship and directed an interdisciplinary research lab for five years. In 2009 he received an Attract Award from the Fraunhofer Society which led him to set up a photonics lab at the Fraunhofer Institute for Physical Measurement Techniques in Freiburg. From 2011-2022 he headed the MPG research group at the Max Planck Institute for Intelligent Systems in Stuttgart, and from 2013-2022 he was a Professor of Physical Chemistry at the University of Stuttgart. In 2022 he moved his labs to Heidelberg University and the MPI for medical Research. Prof. Peer Fischer won an ERC Grant in 2011 and a World Technology Award in 2016. He received an ERC Advanced Grant in 2018. He is a member of the Max Planck – EPFL Center for Molecular Nanoscience and Technology, and the cluster of excellence 3D Matter Made to Order (3DMM2O). Peer Fischer is a Founding Editorial Board Member of the journal Science Robotics and a Fellow of the Royal Society of Chemistry. Professor Fischer has broad research interests including 3D nanofabrication & assembly, micro- and nano-robotics, active matter, interaction of optical, electric, magnetic, and acoustic fields with matter at small length scales, chirality, and molecular systems engineering.

Assembly and Propulsion of Bioinspired Microsystems

Peer Fischer, Heidelberg University, Germany

Simple microorganisms can move in complex media, respond to the environment and self-organize. The field of nano- and microrobotics takes inspiration from nature and strives to achieve these functions in mobile robotic systems of sub-millimeter size. However, building synthetic motors, machines, and robots ‘bottom up’, such that they can mimic biological matter and function autonomously or such that they can be controlled externally, is a fascinating challenge that requires a multidisciplinary approach. It is generally not possible, to directly translate actuation mechanisms and design-concepts from the macro- to the nanoscale. At this scale, different physical phenomena are important and there are no ready-made motors and no off-the-shelf parts. I will discuss nanofabrication and assembly strategies to obtain artificial microswimmers and microrobotic systems, as well as means to actuate and control these. I will also discuss how one may build living machines.

MüSIM2023 Speakers



Prof. Dr. Stefan Hecht

Humboldt-Universität zu Berlin
Center for the Science of Materials
Berlin, Germany

Stefan Hecht was born in 1974 and grew up in Berlin, where he studied chemistry at Humboldt-Universität from 1992-1997. He carried out his Diplom thesis research in the area of organic photochemistry with the late Prof. William G. Dauben at the University of California, Berkeley. After receiving his diploma from Humboldt-Universität zu Berlin in 1997, he returned to Berkeley to pursue his graduate studies in the field of organic polymer chemistry under the guidance of Prof. Jean M. J. Fréchet and obtained his Ph.D. degree in 2001. Directly after, he started his independent academic career as a young investigator (assistant professor) at Freie Universität Berlin (2001-2004) and continued as a group leader (associate professor) at the Max Planck Institute for Coal Research in Mülheim upon Ruhr (2005-2006). From 2006-2019 he held the Chair of Organic Chemistry and Functional Materials at Humboldt-Universität zu Berlin. From August 2019 till December 2022, Prof. Hecht was the Scientific Director of the Leibniz Institute for Interactive Materials (DWI) in Aachen and holds the Chair of Macromolecular Chemistry at RWTH Aachen University. In fall 2022, he started an Einstein Professorship at Berlin's Humboldt University.

Stefan Hecht's research interests are primarily devoted to the development of macromolecular and supramolecular systems and their assembly/integration into materials, able to interact with their environment and respond to specific internal and external stimuli. Particular focus is on the exploration of light-responsive units to optically control and drive biological, chemical, and physical processes to realize unprecedented material properties and achieve new device functions.

Illuminating Materials, Devices, and Manufacturing with Photoswitches

Stefan Hecht, Humboldt-Universität zu Berlin, Germany

Using an external light stimulus to control and power advanced materials and devices thereof in a dynamic fashion with superior spatial and temporal resolution offers tremendous opportunities. In this context, molecular photoswitches that undergo reversible changes upon illumination have become key ingredients. However, to develop these systems into high-performing materials and practical applications the switching processes have to be highly efficient and reliable. Both criteria are stringent and necessitate continuing optimization of key parameters, involving spectral separation and selective addressability in attractive wavelength regions that enable sufficient light penetration, high quantum yields for switching in both directions, enhanced (photo)chemical resistance enabling highly repetitive switching without fatigue, among others. Importantly, the photoswitchable systems of choice have to undergo significant changes of a physicochemical property of choice in order to maximize its overall achievable modulation. This presentation will briefly highlight selected examples from our laboratory to illustrate how progress in molecular design can be directly translated into materials innovation, ranging from remote-controlled (self)healing films and rubbers over photoactuating films and coatings to various optically gated electronic devices in transistors, memories, and displays. Moreover, we have developed photoswitchable photoinitiators that form the basis for a new volumetric 3D printing method – xolography – that we have recently developed. Fiat lux – let there be light!

MüSIM2023 Speakers



Prof. Dr. Rafal Klajn

Weizmann Institute of Science

Rehovot, Israel

Institute of Science and Technology Austria

Vienna, Austria

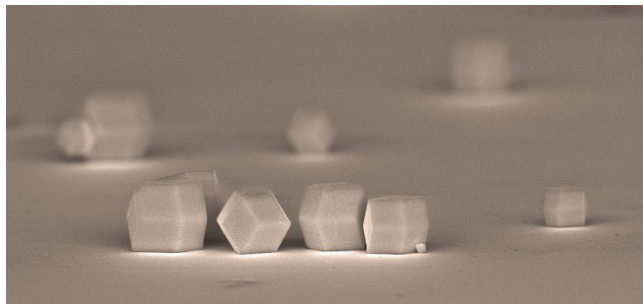
Rafal Klajn completed his undergraduate education and an MSc in Chemistry at the University of Warsaw in 2004. In 2009 he obtained a PhD degree in Chemical & Biological Engineering at Northwestern University. He then joined the Weizmann Institute of Science, where he is currently a full professor. He has served on the boards of several journals, including Chem, ACS Nano, and ChemSystemsChem, and received several awards, including the Netherlands Scholar Award for Supramolecular Chemistry, the Cram Lehn Pedersen Prize in Supramolecular Chemistry, and the Sigma-Aldrich lectureship in Materials Science.

Rafal Klajn is a recipient of several international honors and awards, including the 2010 IUPAC Prize for Young Chemists, the 2013 Victor K. LaMer Award from the American Chemical Society, a 2013 European Research Council (ERC) Starting Grant, the 2015 Liebig Lectureship from the German Chemical Society, the 2015 Israel Chemical Society Prize for Outstanding Young Scientists, the 2016 Netherlands Scholar Award for Supramolecular Chemistry, the 2017 Distinguished Lectureship Award in Photochemistry from the Chemical Society of Japan, the 2017 Chemical Society Reviews Emerging Investigator Lectureship, a 2018 ERC Consolidator Grant, the 2018 Cram Lehn Pedersen Prize in Supramolecular Chemistry, the 2019 Award for Research Cooperation and High Excellence in Science (ARCHES) from the Federal German Ministry for Education and Research, the 2019 New Horizons Solvay Lectureship in Chemistry (International Solvay Institutes), the 2019 Sigma-Aldrich Lectureship in Materials Science, and the 2021 Blavatnik Award for Young Scientists in Israel.

Electrostatic Self-Assembly of Nanoparticles into Static and out-of-Equilibrium Materials

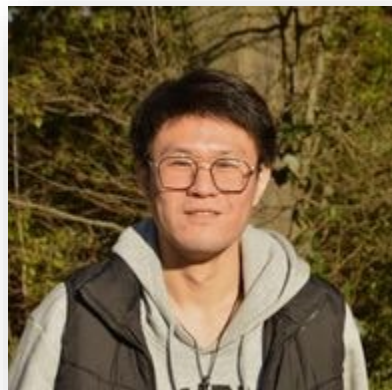
Rafal Klajn, Weizmann Institute, Israel

Self-assembly of inorganic nanoparticles (NPs) into ordered structures (“superlattices”) has led to a wide range of nanomaterials with unique optical, electronic, and catalytic properties. Various interactions have been employed to direct the crystallization of NPs, including van der Waals forces, hydrogen bonding, as well as electric and magnetic dipolar interactions. Among them, Coulombic interactions have remained largely unexplored, owing to the rapid charge ligand exchange between NPs bearing high densities of opposite charges. In this talk, I will describe a new method to assemble such “superionic NPs” under conditions that preserve their native surface charge density. Our



methodology was used to assemble oppositely charged NPs into high-quality superlattices exhibiting Catalan shapes. The methodology can be applied to a wide range of charged nanoparticles of various sizes, shapes, and compositions. I will also discuss two ways to employ electrostatic interactions to assemble NPs into transient assemblies, whose lifetimes depend on and can be controlled by the availability of small-molecule ionic “fuels”.

MüSIM2023 Young Researcher Awardees



Yuhao Ji, M.S.

Institute of Physiological Chemistry and
Pathochemistry
University of Münster
Münster, Germany

For his contribution

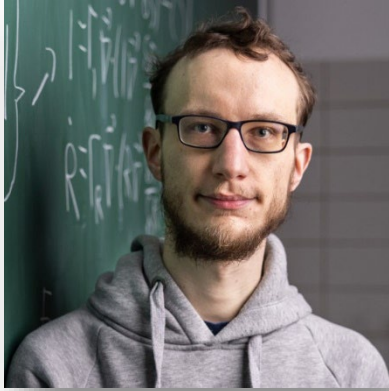
Self-Regulated and Bidirectional Communication in Synthetic Cell Communities

Yuhao Ji, Taniya Chakraborty, and Seraphine V. Wegner

ACS Nano 2023, 17, 10, 8992-9002

Cell-to-cell communication is not limited to a sender releasing a signaling molecule and a receiver perceiving it but is often self-regulated and bidirectional. Yet, in communities of synthetic cells, such features that render communication efficient and adaptive are missing. Here, we report the design and implementation of adaptive two-way signaling with lipid-vesicle-based synthetic cells. The first layer of self-regulation derives from coupling the temporal dynamics of the signal, H₂O₂, production in the sender to adhesions between sender and receiver cells. This way the receiver stays within the signaling range for the duration sender produces the signal and detaches once the signal fades. Specifically, H₂O₂ acts as both a forward signal and a regulator of the adhesions by activating photoswitchable proteins at the surface for the duration of the chemiluminescence. The second layer of self-regulation arises when the adhesions render the receiver permeable and trigger the release of a backward signal, resulting in bidirectional exchange. These design rules provide a concept for engineering multicellular systems with adaptive communication.

MüSIM2023 Young Researcher Awardees



Dr. Michael te Vrugt

Institute of Theoretical Physics
University of Münster
Münster, Germany

For his contribution

From a Microscopic Inertial Active Matter Model to the Schrödinger Equation

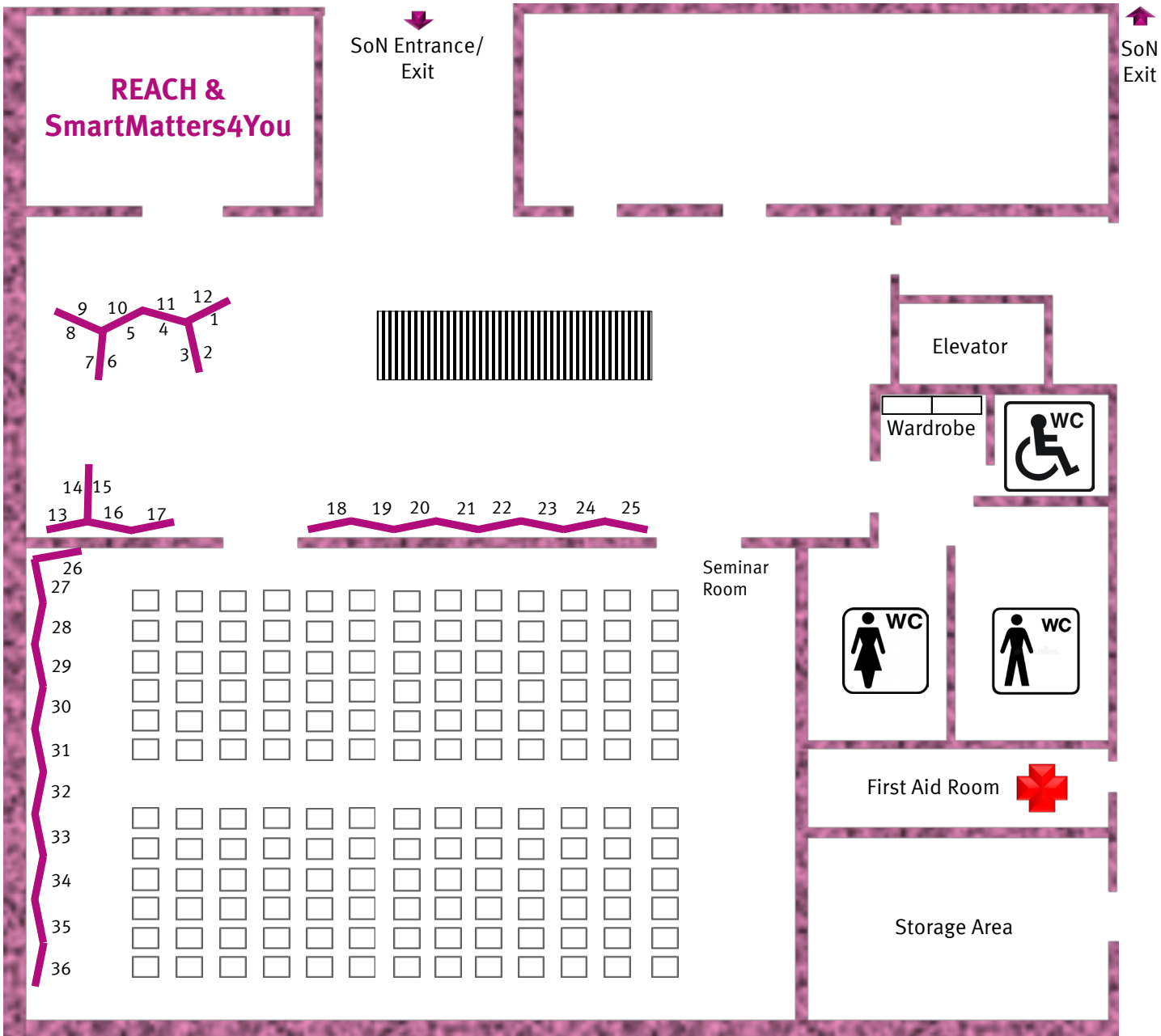
Michael te Vrugt, Tobias Frohoff-Hülsmann, Eyal Heifetz, Uwe Thiele and Raphael Wittkowski
Nature Communications 2023, 14: 1302

Active field theories, such as the paradigmatic model known as ‘active model B+’, are simple yet very powerful tools for describing phenomena such as motility-induced phase separation. No comparable theory has been derived yet for the underdamped case. In this work, we introduce active model I+, an extension of active model B+ to particles with inertia. The governing equations of active model I+ are systematically derived from the microscopic Langevin equations. We show that, for underdamped active particles, thermodynamic and mechanical definitions of the velocity field no longer coincide and that the density-dependent swimming speed plays the role of an effective viscosity. Moreover, active model I+ contains an analog of the Schrödinger equation in Madelung form as a limiting case, allowing one to find analogs of the quantum-mechanical tunnel effect and of fuzzy dark matter in active fluids. We investigate the active tunnel effect analytically and via numerical continuation.



2nd Münster Symposium on Intelligent Matter June 14th, 2023

Poster Sessions Setup



Poster Session I (odd numbers): 1:00pm – 1:50pm
Poster Session II (even numbers): 1:50pm – 2:40pm

MüSIM2023 Poster Contributions

(alphabetical order, first author's surname)

- 01. Manipulating Matter using Light-Induced Virtual Electrodes Based on Lithium Niobate**
Eric Asché, Riccardo Zamboni, Jan ter Glane, Cornelia Denz, and Jörg Imbrock
University of Münster
- 02. Nonlinear Activation Functions in Optical Neural Networks**
Marlon Becker, Jan Riegelmeyer, Maximilian Seyfried, Bart Jan Ravoo, Carsten Schuck, Benjamin Risse
University of Münster
- 03. Integrating Memory into Hybrid Opto-Electronic Circuits**
Ivonne Bente¹, Reinier J.C. Cool^{1,2}, Donato F. Falcone³, Laura Bégon-Lours³, Valeria Bragaglia³, Bert Jan Offrein^{2,3}, Wilfred G. van der Wiel^{1,2} and Wolfram H.P. Pernice^{1,4}
¹University of Münster, ²University of Twente, ³IBM Research Europe – Zurich Research Laboratory, ⁴Heidelberg University
- 04. Self-Assembly of Hybrid Nanostructures for Brain-Inspired Electronics**
Marc Beuel^{1,2}, Jonas Mensing¹, Lisa Schlichter¹, Andreas Heuer¹, Bart Jan Ravoo¹, and Wilfred van der Wiel^{1,2}
¹ University of Münster, ²University of Twente
- 05. Dynamic Molecular Switches Based on HATNA Derivatives for Application in Neuromorphic Computing**
Alessandro Borrini, Christian A. Nijhuis
University of Twente
- 06. Accumulation and Identification of Micro- and Nano-Plastics Dispersed in Water by Optoelectronic Platforms**
Pablo Camarero, Carlos Sebastián-Vicente, I. Ferre-Martín, Patricia Haro-González, Ángel García-Cabañes and Mercedes Carrascosa
Universidad Autónoma de Madrid
- 07. Controlling the Hierarchical Assembly of Vesicles Using Multivalent Interactions**
Krishnendu Das and Jurriaan Huskens
University of Twente
- 08. Exploiting the Interplay of Multiple Independent Stimuli: Designing a Ratchet-Like Process**
Torsten Dünnebacke, Niklas Niemeier, Sebastian Hochstädt, Gustavo Fernandez, Johannes Neugebauer, Michael Ryan Hansen
University of Münster

MüSIM2023 Poster Contributions

(alphabetical order, first author's surname)

- 09. Multistimuli Responsive Materials with Memory and Feedback Function**
Saskia Frank, Alice Casadidio, and Seraphine V. Wegner
University of Münster
- 10. Adaptive Air-Water Interfaces with Spiropyran and Arylazopyrazole Photoswitches**
Michael Hardt^{1,2}, H.Gökberk Özcelik¹, David Bienek¹, Andreas Heuer¹, Björn Braunschweig^{1,2}
University of Münster
- 11. Synthesis and Characterization of a Reporter Molecule for Optical Voltage Sensing**
Meike C. Höhl, M. Victoria Cappellari, Cristian A. Strassert, Anna Junker
University of Münster
- 12. Light-Controlled Anion-Binding Adaptive Supramolecular Systems**
Leon Hoppmann, Leonard Wyszynski, Olga García Mancheño, Monika Schönhoff
University of Münster
- 13. Photoinhibitors of Urease Enable pH Control in Enzymatic Networks**
Nikita Ivanov, Alexandar Slivkov, Wilhelm Huck
Radboud University
- 14. Self-Regulated and Bidirectional Communication in Synthetic Cell Communities**
Yuhao Li, Taniya Chakraborty and Seraphine V. Wegner
University of Münster
- 15. Poly-L-Lysine-Coated Microfluidic Channels Enable Communication with Chemical Reaction Networks**
Alive Hazal Kovuncu, Jacopo Movilli, Dimitrii V. Kriukov, Jurriaan Huskens, Albert S.Y. Wong
University of Twente
- 16. Logical Machine and Noise Filter in Autocatalytic Chemical Reaction Network**
Dmitrii V. Kriukov, Albert S.Y. Wong
University of Twente
- 17. Linear Water (in)soluble Platinum(II) Complexes of a Tridentate Ligand as Selective Guanine Quadruplex Binders**
Simon Kross, Jens Müller
University of Münster

MüSIM2023 Poster Contributions

(alphabetical order, first author's surname)

18. Chirality-Induced Electron Spinpolarization in Chiral Oxide Thin Films

Paul V. Möllers¹, Jimeng Wei², Supriya Ghosh², Soma Salamon³, Manfred Bartsch¹, Heiko Wende³, David Waldeck², Helmut Zacharias¹

¹University of Münster, ²University of Pittsburgh, ³University of Duisburg-Essen

19. Adaptive Cell-Matrix Nanosystems

Theresa Mößer¹, Tobias Rex¹, Inka Schröter², Carsten Grashoff¹, Cristian A. Strassert¹, and Britta Trappmann²

¹University of Münster, ²MPI Molecular Biomedicine

20. Creating Adaptive Liquid Crystals by Dynamic Covalent Chemistry

Torben Neumann, Meik Blanke, and Michael Giese

University of Duisburg-Essen

21. Control of the Primary and Secondary Structure in Synthetic Polymers to Access Adaptive Soft Materials

C. Pauly, K. Markelov, A. Emmerich, P. Gerdt, A. Studer

University of Münster

22. A Semi-Synthetic Nanosystem for Programmable Control of Output Based on Rational Design and Directed Evolution

Aileen Peters, Anna-Maria Böttick, Esther Tanumihardja and Prof. Dr. Andrea Rentmeister

University of Münster

23. Adaptive Polymer Morphologies through Reversible Block Fragmentation

Yorick Post, Katharina Ziegler, André Gröschel, Bart Jan Ravoo

University of Münster

24. Spin Wave Device as a Basis for Neuromorphic Computing

Dmitrii Raskhodchikov¹, Jannis Bensmann¹, Kirill O. Nikolaev², Emma Lomonte¹, Lin Jin¹, Paul Steeger¹, Johann A. Preuß¹, Robert Schmidt¹, Robert Schneider¹, Johannes Kern¹, Steffen Michaelis de Vasconcellos¹, Rudolf Bratschitsch¹, Sergej O. Demokritov¹, Wolfram H.P. Pernice^{1,2} and Vladislav E. Demidov¹

¹University of Münster, ²Heidelberg University

25. Advanced Luminescent Materials: From Optoelectronics to Bioapplications

Fabio Rizzo

University of Münster

MüSIM2023 Poster Contributions

(alphabetical order, first author's surname)

- 26. Light-Driven Microswimmers with a Symmetry-Breaking Refractive Index Profile**
Matthias Rüschenbaum¹, Julian Leggle¹, Elena Vinnemeier¹, Jörg Imbrock¹, Cornelia Denz^{1,2}, and Raphael Wittkowski¹
¹University of Münster, ²Physikalisch-Technische Bundesanstalt
- 27. Signatures for Collective Electronic Excitations between Moiré Bands in Twisted Tungsten Selenide (tWSe₂) Bilayers**
Nihit Saigal¹, Hendrik Lambers¹, Lennart Klebl², Veljko Antic¹, Sina Bahmanyar¹, Tim Wehling² and Ursula Wurstbauer¹,
¹University of Münster, ²University of Hamburg
- 28. Luminescent Oxygen Sensor Based on Platinum(II)-Decorated DNA**
Tim Schäfer, Felix Boisten, Iván Maisuls, Cristian A. Strassert and Jens Müller
University of Münster
- 29. New Photoswitches for the Integration in Adaptive Nanosystems**
Malte Schrader, Florian Bosse, Bastian Stövesand, Bart Jan Ravoo, and Frank Glorius
University of Münster
- 30. Light-Driven Patterning of Electric Charge on Passive Dielectric Substrates using Fe:LiNbO₃ Photovoltaic Stamps**
Carlos Sebastián-Vicente¹, Ángel García-Cabañes¹, Riccardo Zamboni², Jörg Imbrock², and Mercedes Carrascosa¹
¹Universidad Autónoma de Madrid, ²University of Münster
- 31. Functionalization of Piezoelectric Nanoparticles with Arylazopyrazole Photoswitches**
Henri Tertilt, Lisa Schlichter, Michael Holtkamp, Sebastian Hochstädt, Stephan Klemme, and Bart Jan Ravoo
University of Münster
- 32. From a Microscopic Inertial Active Matter Model to the Schrödinger Equation**
Michael te Vrugt¹, Tobias Frohoff-Hülsmann¹, Eyal Heifetz², Uwe Thiele¹, Raphael Wittkowski¹
¹University of Münster, ²Tel Aviv University
- 33. Developing Tunable Triplet Emitters towards Adaptive Electroluminescent Materials**
Tobias Theiss, Dominik Schwab, Alex Oster, Nikos Doltsinis and Cristian A. Strassert
University of Münster

MüSIM2023 Poster Contributions

(alphabetical order, first author's surname)

34. Photo-Responsive HB CLC Films for Digital Photonic Patterning

Tobias Thiele, Florian Malotke, Michael Giese
University of Duisburg-Essen

35. Controlling Imine Formation with Light – A Way to Adaptive Materials

Jana Tietze, Torben Neumann, Michael Giese
University of Duisburg-Essen

36. Towards Electro-Optical In-Memory Computing with Phase Change Materials

Niklas Vollmar¹, Akhil Varri¹, Daniel Wendland¹, Nishant Saxena¹, Wolfram Pernice^{1,2}, Martin Salinga¹

¹University of Münster, ²Heidelberg University

Special MüSIM2023 Contributions

(alphabetical order, first author's surname)

SmartMatters4You: Students Gain Insights into Research at the SFB 1459 "Intelligent Matter"

Julian Repke

University of Münster

REACH EUREGIO Start-up Center - From Science to Start-up

Anne Vortkamp

University of Münster, REACH EUREGIO Start-up Center

MüSIM2023 Poster Abstracts

1

Manipulating Matter using Light-Induced Virtual Electrodes Based on Lithium Niobate

Eric Asché, Riccardo Zamboni, Jan ter Glane, Cornelia Denz, and Jörg Imbrock

*University of Münster, Institute of Applied Physics Corrensstraße 2/4, 48149, Münster,
Germany*

eric.asche@uni-muenster.de

Electric fields are well suited as a tool for actuating micro- and nanoparticles due to the strong dielectrophoretic or electrophoretic interactions. Similarly, light has been used extensively to control and observe matter. The study of active matter benefits from both methods^{1,2}, taking advantage of the simple structuring of light and the strong interaction of the electric field. We present a platform that combines both advantages without the need for additional bulky instrumentation. Virtual electrodes are induced by the light structures onto a ferroelectric crystal of lithium niobate. The latter replaces glass slides in microfluidic devices in a conventional microscope system. Additionally, the strength, shape and time evolution of electric fields can be tuned by shaping the light field spatially and temporally. It is shown that virtual electrodes can manipulate and arrange micro- and nanoparticles of different materials and guide microfluidic droplets in micrometer-sized fluidic channels³.

References:

1. R. Marcel, G. Volpe, and G. Volpe. "Light, Matter, Action: Shining light on active matter." ACS Photonics (2023).
2. Y. Jing, et al. "Reconfiguring active particles by electrostatic imbalance." Nature materials 15.10 (2016).
3. R. Zamboni, et al. "Manipulating aqueous droplets by light-induced virtual electrodes" Optical Trapping and Optical Micromanipulation XVIII 11798 (2021).

Nonlinear Activation Functions in Optical Neural Networks

Marlon Becker^{1,2}, Jan Riegelmeyer^{3,4}, Maximilian Seyfried^{5,6}, Bart Jan Ravoo^{5,6}, Carsten Schuck^{3,4}, Benjamin Risse^{1,2}

University of Münster

¹*Institute for Geoinformatics*, ²*Institute for Computer Science*, ³*Department for Quantum Technology*, ⁴*Center for NanoTechnology*, ⁵*Institute for Organic Chemistry*, ⁶*Center for Soft Nanoscience, Münster, Germany*

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Optical neural networks (ONNs) hold great potential for faster and more energy efficient information processing in coherent photonic circuits than currently possible in electronic processors. Corresponding linear optical operations have already successfully been demonstrated but optical nonlinearities for implementing required activation functions pose a key challenge for practical realizations of ONNs. While some optical nonlinear mechanisms, such as saturable absorption, are known, current implementations do not offer tunability, which will allow for optimizing network performance as well as for understanding the emergence of intelligent behavior in a neural network. Photo-switchable chemical compounds are well studied optically active systems that feature a wide range of configurable photo-physical properties, which have been used for controlling and manipulating conformation and molecular structure. Here we make the nonlinear properties of this large, highly adaptive class of photo-switches accessible as activation functions in optical neural networks. We employ photo-induced isomerization in azobenzenes to steer activation behavior through nonlinear modulation of an information carrying optical signal and control the strength of the nonlinearity via the chemical concentration. We find that a physically motivated model can describe experimental data for systematically varied photo-switching parameters, resulting in a tunable yet interpretable activation function.

Combining Integrating Memory into Hybrid Opto-Electronic Circuits

Ivonne Bente^{1,2,3*}, Reinier J.C. Cool^{1,4,5}, Donato F. Falcone⁶, Laura Bégon-Lours⁶, Valeria Bragaglia⁶, Bert Jan Offrein^{5,6}, Wilfred G. van der Wiel^{1,4,5} and Wolfram H.P. Pernice^{1,2,3,7}

University of Münster, Center for Soft Nanoscience (SoN), Busso-Peus-Str. 10, 48149, Münster, Germany,

²Institute of Physics, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany,

³CeNTech – Center for Nanotechnology, Heisenbergstr. 11, 48149 Münster, Germany,

⁴University of Twente, Faculty of Electrical Engineering, Mathematics and Computer Science, Hallenweg 23, 7522NH, Enschede, The Netherlands,

⁵University of Twente, MESA+ Institute, Hallenweg 15, 7522NH, Enschede, The Netherlands,

⁶IBM Research Europe - Zurich Research Laboratory, CH-8803, Rüschlikon, Switzerland

⁷Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg, Germany

** i.bente@uni-muenster.de*

Combining technologies meant for edge AI applications could enhance the individual technologies strengths and suppress their weaknesses. Low energy and ultra-low latency preprocessing of Photonic Convolution Processors (PCP) combined with the rich processing capabilities of Dopant Network Processing Units (DNPU) is a very promising combination. A first layer of a software neural network is directly built in hardware. The PCP represents the inputs and multiplication by the weight matrix, after which the DNPUs directly perform a tunable non-linear operation. To enhance this system, PCPs and DNPUS are being upgraded to the next generation. The PCPs are enhanced by optimizing its multiplexing capabilities and electronic control. Memory is introduced to DNPUs by means of a ferroelectric layer, greatly improving its energy efficiency and scalability. PCPs with DNPUs could prove to be a promising system for the next generation of AI edge applications.

Self-Assembly of Hybrid Nanostructures for Brain-Inspired Electronics

Marc Beuel^{1,2,3,4}, Jonas Mensing⁵, Lisa Schlichter³, Andreas Heuer⁵, Bart Jan Ravoo³, and Wilfred van der Wiel^{1,2,4}

¹*BRAINS Center for Brain-Inspired Nano Systems and MESA+ Institute for Nanotechnology, University of Twente, Drienerlolaan 5, 7522 NB Enschede, The Netherlands*

²*University of Twente, Faculty of Electrical Engineering, Mathematics and Computer Science, Hallenweg 23, 7522NH, Enschede, The Netherlands*

³*Center for Soft Nanoscience / Organisch-Chemisches Institut, University of Münster, Busso-Peus-Straße 10, 48149 Münster, Germany*

⁴*Physikalisches Institut, University of Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany*

⁵*Institut für Physikalische Chemie, University of Münster, Corrensstraße 28-30, 48149 Münster, Germany*

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We want to achieve reconfigurable computational functionality in a designless nanoparticle network for machine learning applications using artificial evolution in nanoscale materials. Previous research¹ has shown that disordered networks of functionalized nanoparticles can be configured to behave like Boolean logic gates and binary classifiers.

Herein, hybrid organic-inorganic nanostructures based on the assembly of nanoparticle networks connected by junctions composed of tailor-made organic ligands are constructed. Gold nanoparticles act as single electron transistors while organic ligands act as tunable tunnel barriers introducing synaptic, tunable memory. Host-guest complexes with cyclodextrin and various guest molecules are explored as supramolecular junctions. Insulator and semi-conductors as well as molecular switches like arylazopyrazoles that can be addressed with light are studied. By using dip pen nanolithography, the supramolecular networks of gold nanoparticles are deposited on surfaces between nanoelectrodes.

The fabricated devices are measured in a cryostat at ≤ 5 K and a genetic algorithm is used to find suitable configurations of control voltages to mimic the desired computations (Evolution-in-materio).

The theoretical underpinning of nanoparticle networks is investigated by developing a highly optimized physical model to simulate charge transport processes within the network stochastically. Besides, statistical and data-driven tools investigate requirements for computing and memory functionalities.

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Dynamic Molecular Switches Based on HATNA Derivatives for Application in Neuromorphic Computing

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Currently, about 5%–15% of the world's energy is spent in some form of data manipulation and this fraction is expected to rapidly increase. Between 20 and 30 MW are estimated for von Neumann type computers to emulate same level of complexity as our brains. Our brain works with 20 W.¹ Neuromorphic computing architecture focuses on building electronic neural processing systems that directly emulate real neurons and synapses. Currently, most approaches to neuromorphic computing rely on high energy consuming silicon materials.² An attractive energy efficient solution is given by molecular switches which can potentially simulate synaptic plasticity. However, up to now, molecular switches can only switch between fixed on and off states, hence showing a static rather than dynamic behaviour. The key factor to reproduce synaptic plasticity is coupling different processes each characterised with its own time constant, analogues of action potential coupled to slow diffusion of Ca²⁺ and neurotransmitters in synapses. 5,6,11,12,17,18- hexaazatrinaphthylene (HATNA) in a tunnelling junction is a promising candidate because it can couple a fast electron transfer to slow proton transfer.³ Synthetic modification of HATNA with diphenylacetylene (DPA) moieties can potentially facilitate tunneling electron transfer rates in the junction while at the same time enhance packing density of molecules on the electrode.^{4,5} In this poster we give an overview of the synthesis route to achieve the dynamic switch HATNA-DPA and initial monolayer composition studies.

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Accumulation and Identification of Micro- and Nano-Plastics Dispersed in Water by Optoelectronic Platforms

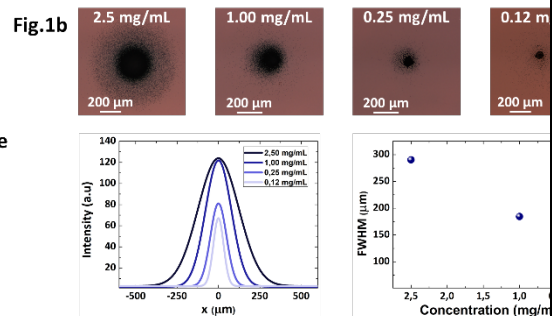
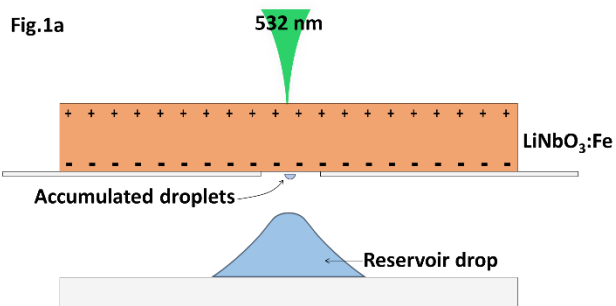
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Plastics pollution in sea and tap water is a main concern in environmental research. In particular, the detection and identification of small size particles (at the micro- and nanoscale) is an important technical challenge and so, several methods are currently investigated to face it. Here, we present an optoelectronic platform based in the high light-induced electric fields generated by the bulk photovoltaic effect in $\text{LiNbO}_3:\text{Fe}$ [1], a reference ferroelectric material. To operate, a water drop is deposited on a slide placed under the crystal at ~ 0.5 - mm-distance (fig.1a). When a laser beam is focused on the crystal, the photo-generated electric field induces the ejection of a high number of droplets from the reservoir drop. These droplets reach the illuminated crystal surface area and evaporate leaving and accumulating the particles, with a roughly gaussian density distribution. First results, showing the successful accumulation of two sizes (1 μm - and 100-nm-diameters) polystyrene and 4- μm -diameter polymethacrylate particles will be reported. Fig.1b shows the microphotographs and density distributions of the 1- μm -polystyrene particles versus the plastic concentration of the mother droplet. The identification of the different kind of plastic particles by Raman spectroscopy will be also discussed.



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Controlling the Hierarchical Assembly of Vesicles Using Multivalent Interactions

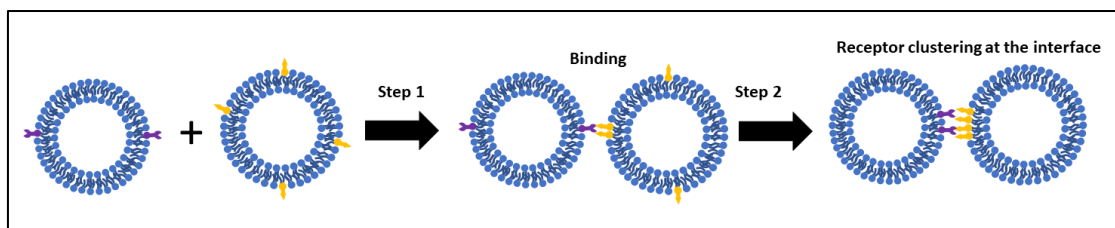
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Keywords: *Multivalency, Vesicles, self-assembly*

From an evolutionary perspective, it is still a long way to answer the question: Why and how did *Life* evolve to multicellular systems, having a higher order of complexity than their unicellular ancestors?^[1] Living systems do not operate in isolation, cells remain attached to each other either directly or via the extracellular matrix through integrins, cell surface proteins, junctions, desmosomes and other interaction motifs, and the collective behavior of the cells expresses the macroscopic life on earth.¹ Biological cells, in a community form have shown better defensive mechanisms against predators, more efficient chemotaxis to find food, and create more efficient functions by dividing tasks between different cells.^{1,2} Therefore, it is intriguing to develop controlled artificial cellular communities by using synthetic vesicles towards exploring the advantages of biological system within chemical framework. This may provide insight into the mechanism of cellular communication and open up new directions on developing *life-like* materials. Therefore, in the present work we demonstrate how multivalent effect can act as a controlling handle to regulate the hierarchical assembly of vesicles. We developed a vesicle-based simplistic model system where two vesicles are engineered to attach to each other through complementary receptors mediated interactions. The multivalent effect permits the receptor clustering at the interface of two vesicles through recruitment.³ Changing the receptor concentration within the individual vesicles enables to control the binding stoichiometry of the vesicles within the hierarchical assembly.



Scheme 1. Schematic illustration of the receptor mediated dimerization of vesicles

We envisage that this work will provide insight into the construction principles of lipid vesicle-based artificial cells. Thereby, it will unfold new scopes of developing lipid vesicle-based artificial biomaterials such as cellular communities or artificial tissues where also vesicles (acting as artificial cells) need to stick to each other for expressing proper shape and function.

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Exploiting the Interplay of Multiple Independent Stimuli: Designing a Ratchet-Like Process

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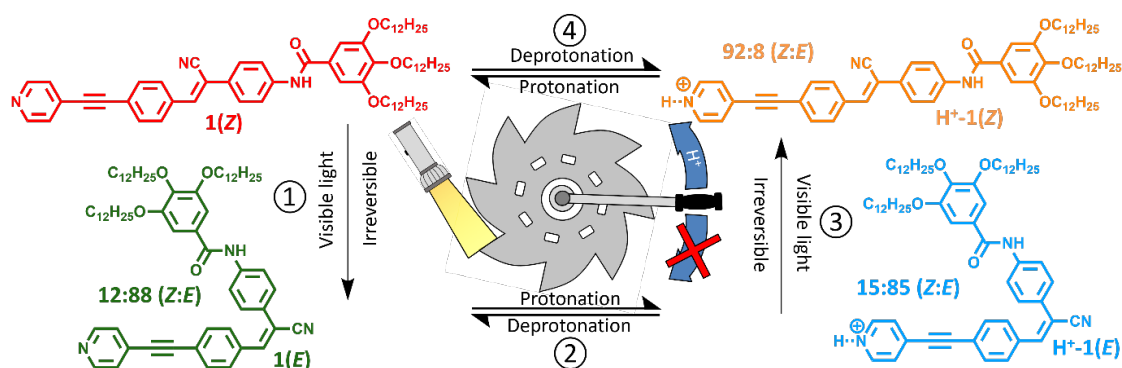
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For the targeted development of responsive and adaptive nanomaterials, fundamental and mechanistic understanding of the interplay between two interdependent stimuli of different nature on the responsiveness of a supramolecular system is required.¹ To study the interdependence of two external stimuli on the responsiveness of a supramolecular building block, a discrete π -conjugated system with two stimuli active entities was designed. A pyridine (pH-response)² and a cyanostilbene (light-response)³ moiety is connected via acetylene bond and combined with an amide that was introduced to enable intermolecular H-bonds in the aggregated state.

Up to this point it is possible to demonstrate that the outcome of a certain stimulus response can nearly entirely change direction depending on whether a second stimulus is present or not, imitating a ratchet-like process. To elucidate the underlying stimulus-responses and the adaptive behavior, a variety of spectroscopic (UV-vis, Luminescence, IR) techniques are used. To facilitate efficient calculations for characterizing supramolecular structures, novel theoretical methods have been developed, significantly broadening the scope and applicability of existing quantum-chemical tools.⁴ Furthermore, a novel *in-situ* spectroscopic NMR setup under MAS conditions was introduced to monitor any molecular changes upon UV/Vis irradiation. Utilizing advantages of solid-state NMR pulse sequences and HR-MAS we will be able to perform (real) time- and temperature-dependent studies for solid aggregates and aggregates in different solvents.

At the current stage of our research the adapted responses of mutually applied stimuli in monomeric vs. aggregated state are under close investigation.



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Multistimuli Responsive Materials with Memory and Feedback Function

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A multiresponsive soft material must be able to sense diverse external stimuli (inputs), process them following a defined chemical logic and adapt its properties (output) accordingly to interact with its environment. Here, we use hydrogels as straight forward soft material as they alter their physical properties upon changes in their internal structure. To achieve multiresponsiveness, photo-switchable proteins, which react toward light of different wavelengths and metal-coordination complexes, which are sensitive to redox potential changes and the presence of small soluble molecules will be used as crosslinks.

While some inputs generate temporary and dynamic responses in the system, input signals that trigger irreversible reactions will lead to the development of a permanent memory and an altered response to subsequent stimuli. Bioluminescence for activation of photoswitchable proteins introduces feedback to the system.

Adaptive Air-Water Interfaces with Spiro-Pyran and Arylazopyrazole Photoswitches

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Interfaces that respond to stimuli such as light or temperature are of great interest for new intelligent materials. Using molecular switches that respond to orthogonal triggers, the properties of fluid interfaces can be preconditioned and a low level of adaptivity can be integrated that extends the possibilities of soft matter interfaces beyond responsive functions.

In this contribution, we report on the adaptive behavior of air-water interfaces that are decorated by spiropyran (SP) and our recently reported arylazopyrazole (AAP) photo-responsive surfactants.^{1,2} The SP surfactants increase their surface activity when irradiated with UV light that causes a ring-closure reaction. *E/Z* photo-isomerization of the AAP surfactants drives a substantial decrease in surface activity and thus desorption from the interface when the AAP surfactants are switched from their *E* to the *Z* state. In addition, at low pH the short thermal lifetime of the *Z* state as well as of the SP form offers the use of thermal relaxation as an alternative trigger. Interfacial properties and molecular kinetics were studied in detail using surface tensiometry and vibrational sum-frequency generation (SFG). These experiments are complemented with classical molecular dynamics simulations of the AAP surfactants that provide a visualization of the occurrences at the air water interface in dependency of the surface coverage.

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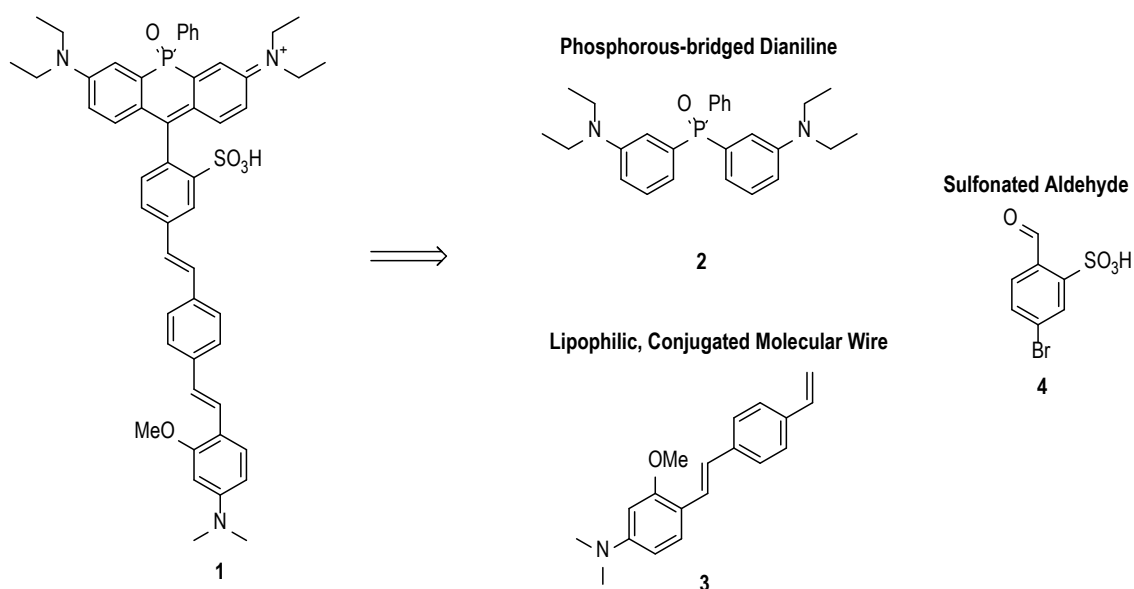
Synthesis and Characterization of a Reporter Molecule for Optical Voltage Sensing

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NIR-absorbing phosphorous-substituted rhodamine dyes (POR) were shown to have outstanding properties as labelling agents in long-term and deep tissue imaging due to their high chemical and photochemical stability, surpassing that of their oxygen- and silicon-substituted counterparts.^[1,2,3] In this work we report the synthesis of phosphorous rhodamine dye **1** for optical voltage sensing bringing together the advantages of POR dyes in terms of stability and NIR excitation with the functionality gained by the introduction of a lipophilic, conjugated molecular wire **3**.



The final POR dye **1** is designed to intercalate into the cell membrane in a manner that the electron donating dimethylamine reaches into the cell membrane enabling voltage sensing while the charged POR head of the molecule prevents cellular uptake. The photophysical characterization of dye **1** in terms of absorption, emission, fluorescence quantum yield ϕ_F and fluorescence lifetime τ_0 is reported in organic media as well as in a buffer system for biological applications.

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Light-Controlled Anion-Binding Adaptive Supramolecular Systems

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Supramolecular hosts featuring 1,2,3-triazoles are known for the cooperative binding of a variety of anions via hydrogen bonds. In previous studies the binding and folding mechanism of a tetra-triazole host was investigated by experimental and theoretical methods like NMR titrations and DFT computations.¹ The structure of the host was further modified by including a light switchable unit (azobenzene or AAP) which can effectively switch between its cis and trans conformation. In NMR titrations with a self-built two-LED in-situ irradiation setup the binding constant of tetrabutylammonium chloride (TBA-Cl) to the host reveals a stronger binding to the cis-isomer. Further refining the host structure by introducing different linkers between the triazole-units yield new azo-triazole hosts with either a chiral cyclohexyl or an achiral aromatic backbone. Successful synthesis pathways were also developed for introducing 1,2- or 1,3-spacing within the aromatic linking units, thus broadening the variety of available hosts. Ongoing optimization aims at enlarging the binding strength difference between the isomers to gain a light-switchable binding behavior.

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Photoinhibitors of Urease Enable pH Control in Enzymatic Networks

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Artificial enzymatic reaction networks are an excellent tool for designing responsive materials and coupling controlled dynamics to chemical functions. In order to tune the enzymatic activity by a light input, one can use photoswitchable inhibitors. Ideally, one of the photoswitchable isomers serves as a strong inhibitor and another is weak. Until now, the progress in the field has been limited by two factors: low differences in inhibitory activities of the two isomers, and the necessity to develop an inhibitor for every particular enzyme.

In the current work, we design photoinhibitors of an enzyme urease to address both issues. Urease catalyzes hydrolysis of urea to ammonia, which leads to rise in pH from 4-5 to 8, thereby increasing the enzyme activity in an autocatalytic manner.

We synthesized a panel of azobenzene-modified urea analogs and found several photoinhibitors of urease. We demonstrate that, due to high sensitivity of the autocatalytic reaction, even moderate difference in the inhibitory properties of the two forms leads to large differences in enzyme kinetics. With use of pH as a versatile handle, this time-controlled behaviour can be coupled to a vast range of functions.

Self-Regulated and Bidirectional Communication in Synthetic Cell Communities

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Cell to cell communication is not just limited to a sender emitting a signalling molecule and a receiver perceiving it but often is two-way and self-regulated, which renders the exchange more efficient and adaptive. In synthetic cells such feedback mechanisms are still missing. Here, we report two-way and self-regulated communication between two populations of synthetic cells, which allows the cells to exchange signals efficiently, when they produce the signal and later separate once the signal diminishes. Specifically, the sender cell produces H₂O₂, which both acts as a signalling molecule and activates chemiluminescence-induced adhesions between the two populations. These adhesions bring sender and receiver in close proximity; simultaneously enhance the transmission efficiency of the signal to the receiver and trigger the release of a feedback signal from the receiver to the sender. The chemiluminescence activation of the adhesions couples the temporal dynamics of signal production in the sender to the spatial proximity to the receiver and once the H₂O₂ signal diminishes, the synthetic cells detach from each other. The feedback between the different molecular elements thereby dynamically alter the communication and the formation of multicellular structures. As a result, there is efficient forward signalling, adaptive backward communication and temporally coupled multicellularity in this community. This model of self-regulated bidirectional communication between synthetic cell provides a roadmap for engineering multicellular systems with adaptive communication.

Poly-L-Lysine-Coated Microfluidic Channels Enable Communication with Chemical Reaction Networks

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In this work, we report a method to create reactive surfaces in microfluidic channels, providing an additional control element for the design of chemical reaction networks (CRNs). This work is inspired by how living systems process information, which can dynamically regulate effective concentrations of chemical components in biological pathways (e.g., in signaling, protein, and metabolic networks). Here, we create reactive surfaces, by coating microfluidic channels with poly-L-lysine (PLL), to exploit its capacity to process information carriers (with units defined as protons). We demonstrate that PLL coated channels provide longer delays compared to uncoated channels, when subjected to a straightforward acid-base reaction based on proton exchange. We developed a mathematical model to explain how this delay can be facilitated by the flow rate (a global transport parameter) and the concentration of an indicator molecule, which in our case is phenol red (which effectively acts as a transmitter). The observation that a local surface-liquid interface enables an overall nonlinear response could provide new ways to develop chemical feedback loops (e.g., local reactions), with a potential to develop CRNs capable of molecular information processing.

Logical Machine and Noise Filter in Autocatalytic Chemical Reaction Network

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Living matter among the diversity of its organization patterns contains intricate chemical reaction networks (CRNs) that process temporal chemical information history-dependently.¹ Design of artificial CRNs for development of life-like adaptive chemical systems is what we investigate in this work. We keep autocatalytic enzyme-based CRN in a stirred flow reactor out of equilibrium to extend its dynamics and controllability. The CRN we use for our studies consists of trypsinogen autocatalysis to trypsin, degradation of both proteins, and control parameters: Ca^{2+} , Nd^{3+} , La^{3+} ions that influence velocity of reactions in the network. Typically, Ca^{2+} is used as a co-factor for trypsinogen autocatalysis because it prevents degradation of both proteins, whereas Nd^{3+} and La^{3+} promote it. Ca^{2+} speeds up autocatalysis, La^{3+} does it more effectively, and Nd^{3+} speeds it up a biphasic way. We demonstrate AND, OR, XOR, NOR, and NAND gating of $[\text{trypsin}]_t$ outflow by two $[\text{Nd}^{3+}]_0$ inputs. When temporal $[\text{Nd}^{3+}]_0$ input changes fast, hysteresis occurs, what enables history-dependent $[\text{Nd}^{3+}]_0$ input processing.² We use $[\text{La}^{3+}]$ -CRN as a Schmitt trigger for temporal changes in $[\text{soybean trypsin inhibitor}]_0$ input. In sum, we program inherent computational functionality of CRN by modulating velocity of reactions inside network with differently acting cofactors of trypsinogen autocatalysis.

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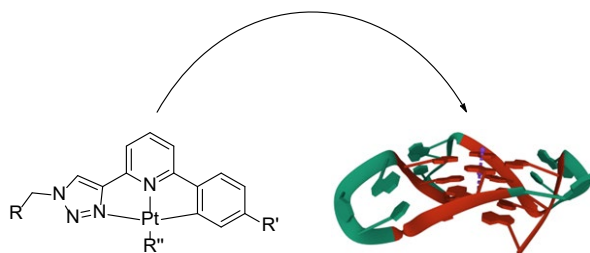
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Linear Water (in)Soluble Platinum(II) Complexes of a Tridentate Ligand as Selective Guanine Quadruplex Binders

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Guanine quadruplex (G4) structures comprise guanine tetrads. Each G tetrad consists of a square-planar arrangement of four guanine residues involved in hydrogen-bonding interactions using their WATSON-CRICK and HOOGSTEEN faces. Two or more guanine tetrads stack upon each other to form a four-stranded helical structure. Guanine-rich sequences are present in the human genome and are known to adopt G quadruplex structures, e.g., in the promoter region of several oncogenes (*c-myc*, *c-kit*) and in telomeres. G quadruplexes play a significant role in the regulation of cell ageing, the transcription of genes and hence emerged as a promising drug target.¹ Especially designed metal complexes could serve as such drugs due to their electronic properties and planar aromatic ligands. Compared to the free ligands, metal binding decreases the electron density of the ligand, thereby increasing the possibility of a π -stacking interaction with the electron-rich G tetrad. Our complexes are based on a functionalized tridentate N^NC ligand. Variation of the substituents (R and R') can introduce functionalities for an enhanced interaction with the G quadruplex.² In continuation of the work by GUHA *et al.*, new luminescent platinum(II) complexes were designed for a selective interaction with G4-DNA.³ The ancillary monodentate ligand in the fourth coordination site (R'') of the platinum ion was used to introduce an additional residue for π -stacking or electrostatic interactions.

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Chirality-Induced Electron Spin Polarization in Chiral Oxide Thin Films

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Spin-polarized catalytic surfaces can greatly enhance the selectivity of chemical reactions, e.g., in a photoinduced water splitting process. Here, we confirm that spin-polarized currents can be obtained from chiral cupric oxide¹ (CuO) and cobalt oxide² (CoOx) layers, and explore the underlying mechanism. Thin chiral oxide layers were deposited using a method pioneered by Switzer et al.³ Photoelectrons were excited with deep-UV laser pulses and their average longitudinal spin polarization (SP) was measured.

For CuO thin films, correlating the SP values with electron energy spectra reveals that the measured SP values could be rationalized assuming an intrinsic SP in the chiral oxide layer and a chirality-induced spin selectivity (CISS)-related spin filtering of the electrons.⁴ On chiral CoOx layers, the SP was found to depend on the Co oxidation state, which allows for reversible switching of the preferred spin orientation. The results support efforts towards a rational design of further spin-selective catalytic oxide materials.

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Adaptive Cell-Matrix Nanosystems

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The aim of our project is the generation of a conceptually novel, biosynthetic material in which mammalian cells are utilized as information-processing elements that sense, integrate, and feedback on mechanical stimuli. One potential read-out parameter is the measurement of mechanical forces with a biological tension sensor, containing a FRET pair of fluorophores. The current tension sensor module is limited by a comparably small signal-to-noise ratio, which aggravates the readout in complex environments. Therefore, we want to explore new coordination-chemical concepts to realize a novel sensor containing a phosphorescent Pt(II) complex as a triplet FRET-donor, which extends the excited state lifetime of the FRET-acceptor from nanosecond (ns) into the microsecond (μ s)-range and thereby enhance the dynamic range of the tension sensor. Finally, these components need to be immobilized on 2D glass surfaces in order to evaluate the applicability of the tension sensor in monitoring extracellular forces.

Creating Adaptive Liquid Crystals by Dynamic Covalent Chemistry

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The relevance of the development of sustainable functional materials is continually increasing. In this context the combination of functionality with adaptivity and reusability is a challenge and focus of research activities. Dynamic covalent chemistry plays a significant role in the field of functional, adaptive and reusable materials e.g. in polymeric networks or molecular cages.¹ But it is rarely used in liquid crystalline materials with adaptive properties.²

In this project we want to use dynamic covalent imine bonds to allow the development of new adaptive and reusable materials in the field of liquid crystals (LC). Since the formation of imines occurs in a dynamic fashion covalent bonds are continually formed and broken. This leads to an adaptive manipulation of the properties and reuse of imine-based materials.^{1,2,3} With the design of LCs based on a library of tailored imines we want to develop materials which can be manipulated by transamination reactions to tune properties such as chirality, fluorescence and the molecular shape of the mesogens.

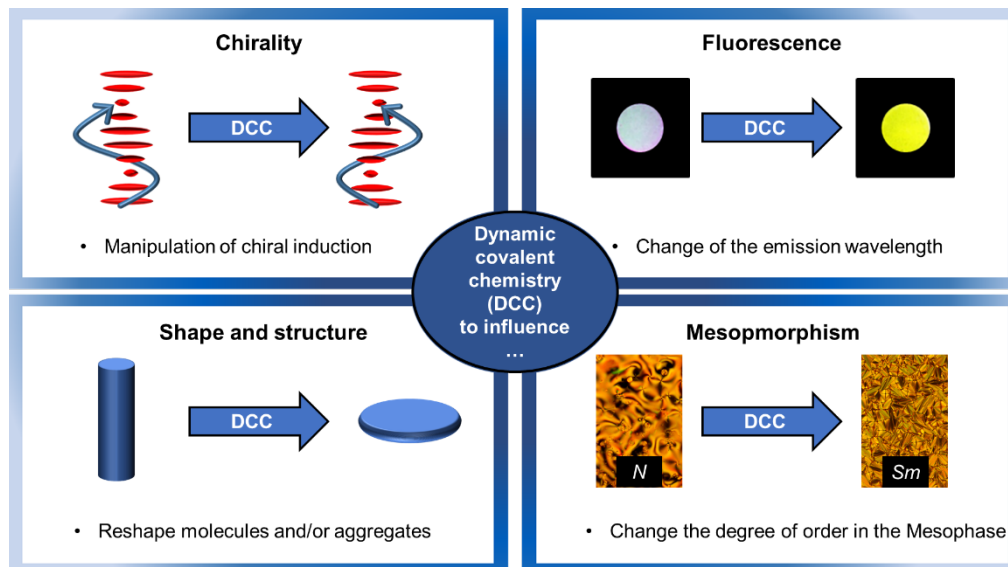


Figure 1. Schematic representation of the different properties which can be influenced by dynamic covalent chemistry

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Control of the Primary and Secondary Structure in Synthetic Polymers to Access Adaptive Soft Materials

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The stereospecific ionic ring-opening polymerization of various donor-acceptor cyclopropanes is reported. The chiral cyclopropane monomers are readily prepared and stereospecific polymerization is conducted with a catalytic amount of MgBr_2 serving as a Lewis acid and as an initiator. Polymers containing a stereocenter in every repeating unit are obtained and the substituents of the monomers can be readily varied to access a novel class of chiral polymers.

A method for the synthesis of functionalized alternating copolymers by reversible deactivation radical polymerization was developed. Copolymerization by reversible addition-fragmentation chain transfer of hexenyl vinyl ether with a novel fluorinated divinyl monomer yields alternating cyclopolymers that can be chemoselectively modified by three distinct orthogonal functionalization reactions.

A Semi-Synthetic Nanosystem for Programmable Control of Output Based on Rational Design and Directed Evolution

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We are engineering a biological system to respond to non-natural fuel (e.g. substrates) and changes of the environment (e.g. light). Integration of feedback loops should help to realize adaptive behavior and self-regulation. Specifically, this means that we aim to change gene expression at the level of transcription or translation in response to AdoMet analogs or their metabolic precursors (i.e. methionine analogs). To achieve this, we synthesize methionine analogs, which can be converted by engineered methionine adenosyltransferases (MATs) to the corresponding AdoMet analogs.^{1,2} MATs are self-regulated by product inhibition through AdoMet (or analogs). This can be circumvented when directly coupling methyltransferases (MTases) to the MAT reaction.³ MTases use AdoMet as cofactor to methylate biomolecules. Usage of promiscuous MTases allows transferring non-natural groups to nucleic acids to regulate their functionalities.⁴ In addition to MAT/MTase cascade reactions, riboswitches can influence gene expression as they actuate protein production when sensing AdoMet,⁵ creating another important output signal depending on the AdoMet level.

Moreover, we are currently establishing microfluidics in our lab, which allows us to minimize the reaction volume to picolitre dimensions and therefore is suitable for various high-throughput screening applications.⁶

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Adaptive Polymer Morphologies through Reversible Block Fragmentation

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Supramolecular structures, which can be operated out-of-equilibrium, are extremely interesting for the development of intelligent materials.¹ In this project, we aim to design a block copolymer that is able to dynamically alter its composition through energy-driven supramolecular fragmentation. Our polymer system consists of two different parts, which are connected through host-guest chemistry. The first part is a block copolymer including the hydrophobic, amorphous poly(methyl methacrylate-co-hexyl methacrylate) (PMH) with low M_n and tuneable glass transition temperature, as well as a short, hydrophilic poly(oligo(ethylene glycol) methacrylate) (POEGMA) with a β -cyclodextrin (β -CD) host molecule as end group. The second part is a longer hydrophilic POEGMA homopolymer with an arylazopyrazole (AAP) guest molecule as end group.

Connecting our two different polymers with this host-guest complex, it will be possible to create reversible micelle morphologies. Driven by a difference in binding affinity of the different photoisomers of AAPs, irradiation by light allows a reversible dissociation. The *E*-isomer can form a host-guest complex with the β -CD, while the binding affinity of the *Z*-isomer is too low for that.²

With this polymer system we want to develop dissipative block copolymer nanostructures, which can potentially form out-of-equilibrium morphologies.

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Spin Wave Device as a Basis for Neuromorphic Computing

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In recent years, it has been shown that spin waves propagating in magnetic guiding structures provide a wide range of possibilities for the implementation of advanced nanoscale devices, including networks for nonBoolean data processing¹ and neuromorphic computing circuits². We use microfocus Brillouin-light-scattering spectroscopy to directly visualize the propagation and transformation of spin waves in a magnetic cross composed of two 800-nm-wide YIG waveguides intersecting at a right angle³. We show that, depending on the frequency, spin waves can experience predominant reflection from the intersection region with weak tunneling of the wave in the forward direction, an efficient redirection of the wave into the side arms of the cross, or almost uniform splitting of the wave into all three arms.

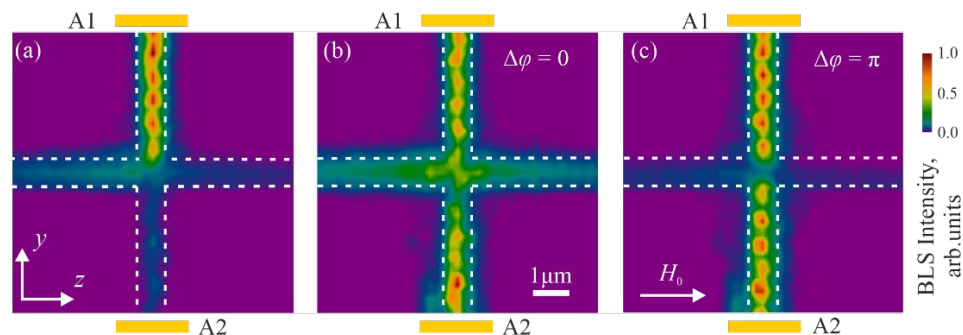


Figure 1: Representative spatial maps of spin-wave intensity recorded at different excitation frequencies.

The observed controllability is useful for steering the propagation of spin waves in complex nanoscale magnonic networks for the implementation of nontraditional computing and signal processing. The high sensitivity of the propagation regime to the frequency of spin waves provides additional opportunities for the manipulation of spinwave propagation by nonlinear effects, such as an amplitude-dependent shift of the spinwave spectrum. This opportunity is particularly important for the realization of neuromorphic networks, where the nonlinear response plays a key role.

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Advanced Luminescent Materials: from Optoelectronics to Bioapplications

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Luminescent materials find applications in many fields, such as solar cells, molecular electronics and bioapplications, depending on the molecular design and the photophysical properties.

Our main motivation is the conceptual development of design motifs to achieve the desired properties of organic emitting molecules for a given application. For this reason, our highly interdisciplinary research lies at the interface between the classical organic chemistry, photophysics and materials science.

Here, we present novel highly emitting organic dyes realized in the group for application in optoelectronics and biosensing.

Light-Driven Microswimmers with a Symmetry-Breaking Refractive Index Profile

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A popular class of active matter are systems of self-propelled particles where energy is supplied externally by optical means. Typically, this is achieved optothermally by inducing a thermal gradient in the medium around each particle which in turn produces a flow field propelling the particle. However, it is also possible to directly transfer momentum from the light field to a microparticle, e.g., via plasmonic resonance. Here we present a mechanism of direct momentum transfer via light refraction. This approach only requires the material of the particles and the solvent to be transparent and to possess a sufficiently large difference in refractive index. The required symmetry breaking for directed particle motion can be achieved both via shape asymmetry or refractive index gradients. We expect that the interplay of non-equilibrium particle dynamics and light refraction will give rise to interesting applications in photonic information processing and is thus a promising candidate for intelligent soft matter.

From a theoretical perspective the interaction between light and particles is modeled as a problem of geometric optics. We present numerical solutions of this model obtained using specialized ray tracing simulations.

For the experimental realization of these particles we employed femtosecond laser lithography by two-photon polymerization yielding high precision and flexibility. We demonstrate experimentally the propulsion of microswimmers with asymmetric shapes and their directional movement.

Signatures for Collective Electronic Excitations between Moiré Bands in Twisted Tungsten Selenide (tWSe₂) Bilayers

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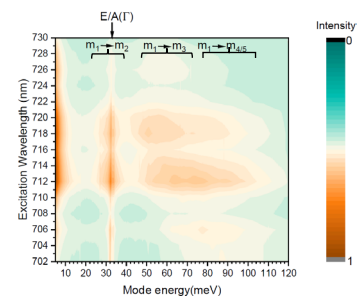
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Twisted bilayers of transition metal dichalcogenides (TMDCs) have emerged as a fertile ground for exploring many body physics and correlated electronic phases such as superconductivity, Mott insulators, Wigner crystals, and excitonic insulator to name a few.¹ The moiré superlattice potential in such systems leads to carrier localization and emergence of (flat) moiré bands in the electronic band structure.² Although the signatures of the flat bands have been shown in STS³ and ARPES⁴ experiments, the observation of electronic transition between them, proving the emergence of those bands, have remained elusive.

We have fabricated hBN encapsulated bilayers of WSe₂ with a twist angle of $\sim 3^\circ$ between the monolayers. In low temperature (4K) resonant inelastic light scattering (RILS) spectra from these bilayers, clear signatures for collective electronic excitations in the energy range between 20meV and 100meV appear in addition to phonon-lines. These strong RILS modes are interpreted as single-particle (SPE) like inter-moiré band excitations analogous to the well-established intersubband electronic excitations from RILS in doped GaAs quantum well structures^{5,6}. Quantitative comparison with calculated moiré band structure of the system supports this interpretation. We discuss the impact of photo-excited charge carrier density (holes) as well as the resonance conditions on SPE-like inter-moiré band transitions as sketched in the figure. We acknowledge support by DFG via WU 637/7-1 and SPP2244.

Fig. RILS spectrum of tWSe₂



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Luminescent Oxygen Sensor Based on Platinum(II)-Decorated DNA

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Nucleic acids represent excellent scaffolds for a programmable three-dimensional arrangement, making use of their modular composition, their facile modification and their superb self-assembly.¹ In this context, the site-specific incorporation of transition metal complexes is of high interest as it can endow the DNA with metal-based properties such as luminescence.²

Towards this end, we utilized the site-specific covalent incorporation of phosphorescent Pt(II) complexes into DNA duplexes. These complexes are derived from a recently established family of Pt(II) complexes containing a tridentate N[^]N[^]C donor ligand and an ancillary monodentate ligand. They show robust phosphorescence, with an emission wavelength essentially independent of the identity of the monodentate ligand. Interestingly, in the case of consecutive complexes within the DNA strand, monomer-based emission is oxygen-sensitive, making the nucleic acid an excellent candidate for oxygen-sensing applications.²

Currently the aim is to establish such an application in biological models and to develop Pt(II) complexes with shorter linkers, so that their location within the DNA can be controlled more precisely.

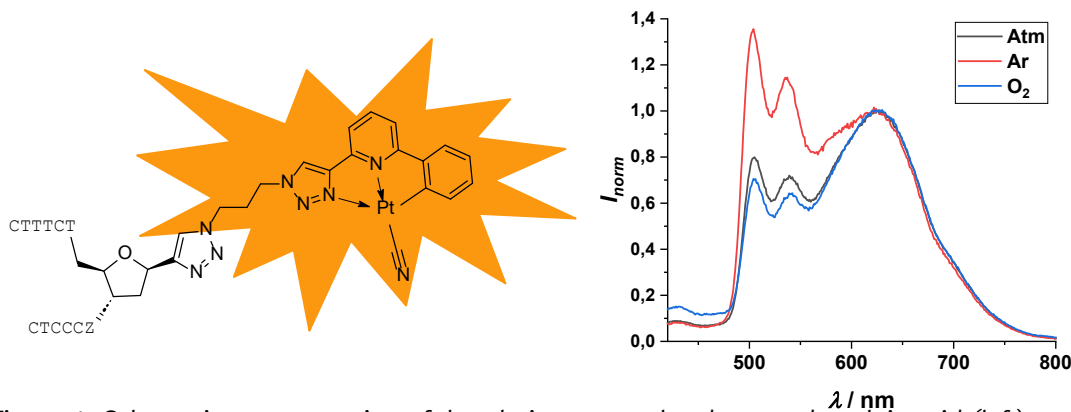


Figure 1: Schematic representation of the platinum-complex-decorated nucleic acid (left) and the corresponding luminescence spectra (right) of the investigated duplex under air-equilibrated conditions (Atm), in argon-saturated solution (Ar) and in oxygen-saturated solution (O₂).

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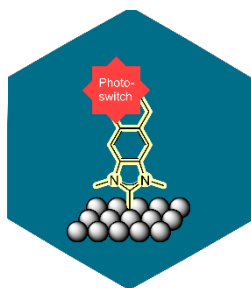
New Photoswitches for the Integration in Adaptive Nanosystems

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Molecular photoswitches are versatile sensors and actuators for the development of intelligent matter. For the assembly of adaptive nanosystems, we design novel photoswitch-building-blocks. Using conjugated *N*-heterocyclic carbene motifs, these will be immobilized on nanoparticles and patterned on surfaces using soft lithography. Furthermore, the developed photoswitches will be integrated in a range of adaptive molecular systems, soft materials and solid-state nanosystems.

Light-Driven Patterning of Electric Charge on Passive Dielectric Substrates using Fe:LiNbO₃ Photovoltaic Stamps

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Unlike metals or semiconductors, dielectric materials allow for the storage of charge patterns for long times thanks to their low electrical conductivity. These charge patterns have many applications: electrostatic assembly of micro/nanoparticles (e.g. laser printers), spatial modulation of wettability, manipulation of liquid droplets, etc. In that context, LiNbO₃ is an outstanding platform where one can generate tailored space-charge distributions by optical and/or thermal stimuli, exploiting the bulk photovoltaic effect and/or the pyroelectric effect. Here, we demonstrate a novel technique for transferring photovoltaic charge patterns from Fe:LiNbO₃ to different passive dielectric substrates (glass, quartz or PMMA). The method resembles the operation of a stamp: 1) first, the Fe:LiNbO₃ crystal is illuminated with the desired light distribution; 2) the crystal is brought into contact with another dielectric substrate; 3) they are separated. As a result, a mirror replica of the original charge pattern is transferred, which we have employed for the dielectrophoretic assembly of micro/nanoparticles (Figure 1) and the dielectrophoretic deformation of thin liquid films. These results establish the foundation of a versatile simple method for charge patterning, tentatively called “photovoltaic charge lithography”.

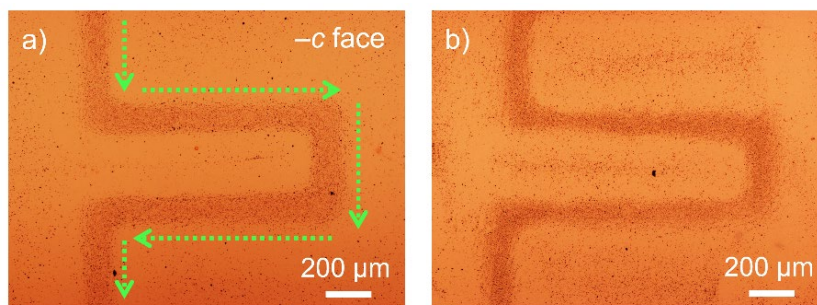


Figure 1. Trapping of Ag nanoparticles along laser beam trajectory (green arrows) on a) z-cut Fe:LiNbO₃ and b) quartz.

Functionalization of Piezoelectric Nanoparticles with Arylazopyrazole Photoswitches

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Piezoelectric materials are important building blocks for modern electronics, sensors and mechanical devices.^[1] Triggering of the piezoelectric effect thereby occurs either by compression on the macroscale, sonication or stress through phase transitions. We propose a new method to possibly trigger the piezoelectric effect indirectly by irradiation through molecular force of photoinduced isomerization. BaTiO₃ nanocrystals and UiO-66 (Zr) MOF nanoparticles were synthesized as piezoelectric anchors with diameters of 10 nm and 100 nm measured by TEM respectively. As photoswitchable bridges between the nanoparticles, arylazopyrazole phosphates (AAPP) were synthesized as good photoswitchable ligands. The surface functionalization of the nanoparticles with monovalent AAPPs was characterized by UV/vis, ICP-OES, ³¹P solid state NMR and XPS. Hence ensuring photoswitchability, a MOF atomic surface functionalization of 60% and the binding between phosphate and Zr. Divalent AAPPs were used to connect the nanoparticles at the liquid-liquid interface and depositions via dip-coating were analyzed by SEM. Ultimately the deposited interfaces will be characterized by conductive AFM regarding the deformation of single particles upon irradiation of the photoswitches. Through the possibility to address piezoelectricity indirectly over molecular force, this method could have potential applications from electronics and sensors to piezocatalysis.

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From a Microscopic Inertial Active Matter Model to the Schrödinger Equation

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Field theories for the one-body density of an active fluid, such as the paradigmatic active model B+, are simple yet very powerful tools for describing phenomena such as motility-induced phase separation. No comparable theory has been derived yet for the underdamped case. In our work, we introduce active model I+¹, an extension of active model B+ to particles with inertia. The governing equations of active model I+ are systematically derived from the microscopic Langevin equations. We show that, for underdamped active particles, thermodynamic and mechanical definitions of the velocity field no longer coincide and that the density-dependent swimming speed plays the role of an effective viscosity. Moreover, active model I+ contains the Schrödinger equation in Madelung form as a limiting case, allowing to find analoga of the quantum-mechanical tunnel effect and of fuzzy dark matter in the active fluid. We investigate the active tunnel effect analytically and via numerical continuation.

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Developing Tunable Triplet Emitters towards Adaptive Electroluminescent Materials

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Functional transition-metal complexes with heavy metal centers such as Pt(II), Ir(III), or Re(I) are well-studied systems because of their photophysical properties and the resulting wide range of applications.¹ Responsive and adaptive systems have increasingly come into focus of research in recent years. Certain properties, such as emission, can be changed (reversibly) by the application of external stimuli such as light, temperature, shear forces or hydrostatic pressure.^{2,3}

In the past months, we have already succeeded in changing the emission of two Pt(II) and Pd(II) complexes by applying shear forces and hydrostatic pressure. A clear red shift can be observed, which can be proven spectroscopically and theoretically. The application of shear forces on crystals of the two complexes causes an irreversible change in emission; hydrostatic pressure, on the other hand, changes the system reversibly.

Density-functional theory calculations suggest that the red-shift occurs due to a shortening of the metal-metal distance in aggregates and a planarization of the complex facilitating a stronger $\pi - \pi$ interaction.

We propose another method leading to a reversible red shift: embedding Pt(II) complexes into photoswitchable polymer microcapsules. Photoswitching leads to a contraction of the capsules, bringing metal centers into closer proximity, enabling dimerization and thus a red shift in energy.

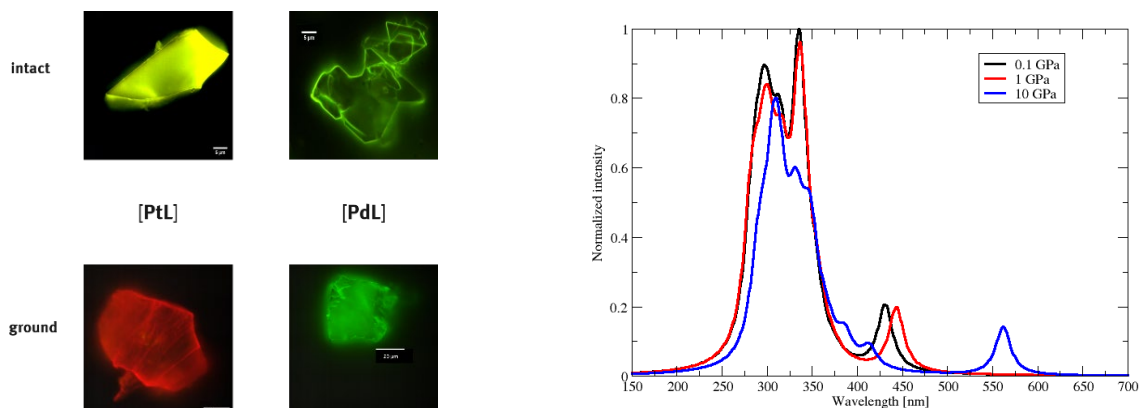


Figure 1. Left: Emissive behavior of the Pt(II) [PtL] and the Pd(II) complexes [PdL] before and after grinding. Right: Calculated absorption spectrum of [PtL] at different pressures.

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Photo-responsive HB CLC Films for Digital Photonic Patterning

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Cholesteric liquid crystals are capable of selectively reflecting circular-polarized light corresponding to the helical pitch of the superstructure.¹ Being able to control the length of the pitch, which results in a change of the reflected wavelength, opens new routes towards holographic data storage technology².

In this project a photoinduced phase transition from a chiral smectic phase to a cholesteric phase was achieved with reflection wavelengths covering the whole range of visible light, representing a full-color display. By irradiating the nearly colorless chiral smectic phase via an SLA 3D-printer any picture or text wanted can be imprinted with a resolution in the micrometer range. The color of the "pixel" is merely determined by the time of irradiation, allowing to imprint any information in one process.

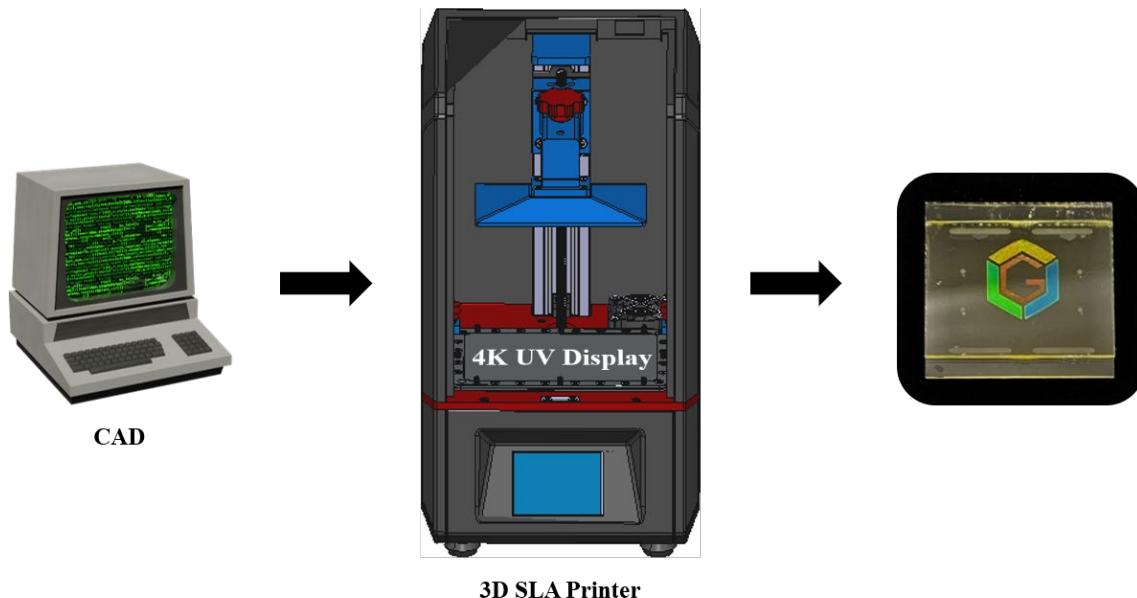


Figure 1: Schematic procedure for imprinting information into a CLC film as a photonic data storage.

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Controlling Imine Formation with Light – A Way to Adaptive Materials

Jana Tietze, Torben Neumann, and Michael Giese

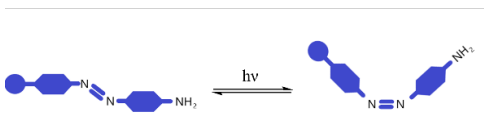
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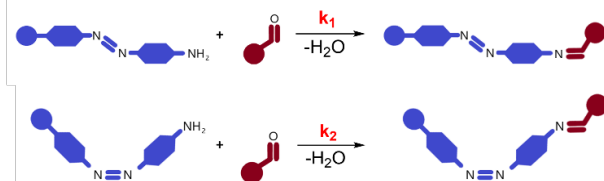
Materials that are responsive to light play a significant role in the development of functional materials, e.g. optical storage devices. The use of photoswitchable azobenzenes is a prominent example for the controlled manipulation of different properties by irradiation with light. Another possibility to influence the properties of functional materials is to employ dynamic covalent chemistry. Both tools were already used in different systems to manipulate mesomorphic behaviour or photophysical properties of liquid crystalline materials.[1][2].

The aim of the project is to use different azobenzene derivatives to manipulate the conversion of dynamic covalent reactions by light. Therefore, we will establish a library of different amino-azobenzene derivatives which we can use in imine based dynamic covalent systems. The photoisomerization of the azobenzene leads to a change in reactivity and has a direct impact on the conversion of imine condensation, transamination and imine metathesis reactions. With this we want to control the properties of imine based liquid crystals by dynamic covalent chemistry with light.

photoisomerization of amino-azobenzene derivatives

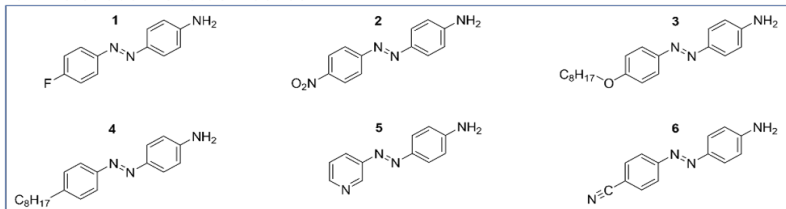


influence of azo-isomerization on imine condensation reactions



molecules used for imine condensation reactions:

amino-azobenzene derivatives



aldehydes

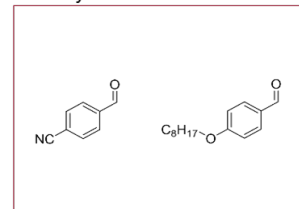


Figure 1: Schematic representation of the photoisomerization of amino-azobenzene derivatives, the influence of the isomerization on the imine condensation reaction and the used amino-azobenzene derivatives and aldehydes.

References:

1. M. Alaasar, *Liquid Crystals* **2016**, 13-15, 2208-2243.
2. M. Blanke, L. Postulka, I. Ciara, F. D'Acerno, M. Hildebrandt, J. S. Gutmann, R. Y. Dong, C. A. Michal, M. Giese, *ACS Appl. Mater. Interfaces* **2022**, 14, 16755–16763.

Towards Electro-Optical In-Memory Computing with Phase Change Materials

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In contrast to von-Neumann processors, in-memory computing systems avoid data movement between a separated processing unit and memory and are therefore fundamentally more efficient in terms of time and energy. In particular, matrix-vector multiplications on crossbar arrays of photonic waveguides can be performed with extremely high throughput, low energy consumption and low latency. A promising approach uses programmable phase-change devices at the crossing points to represent the matrix elements. Depending on the phase configuration of the material, a variable fraction of the incoming light is transmitted. Usually, these phase-change devices are switched with optical pulses, but electrical switching can be advantageous in terms of switching contrast and addressability.

In this project, we develop electro-optical phase-change devices for in-memory computing. Their state is read optically and written with external heating supplied by a microscopic heater. These mixed-mode devices are then implemented into waveguide arrays. Here we present the first steps in the development of the mentioned electro-optical phase-change devices. Additionally, we show experiments on a postprocessing technique that makes a new matrix architecture feasible. This resonator-based architecture offers an advantageous linear loss-scaling. We also show that the developed postprocessing technique is usable to create photonic random access memory units.

SmartMatters4You: Students Gain Insights into Research at the CRC 1459 "Intelligent Matter"

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Since 2019, the number of first-year students in STEM courses has been falling. A particularly strong decline was recorded after the corona pandemic. Aside from the fact that a general recruitment of STEM students is very important for Germany as a technology location, it is particularly important to recruit women for STEM courses. In 2021 only 35% of STEM students in Germany were female¹.

SmartMatter4You empowers scientifically interested female upper school students to pursue a career in science. Through the cooperation from the research in the CRC 1459 "Intelligent Matter" and the know-how of the school laboratory MExLab Physik the students can experience unique access to highly topical research in interdisciplinary workshops and take part in hands-on excursions to science-related companies.

SmartMatters4You helps to bridge the gender gap by raising awareness of gender equality and using empirically proven strategies for success². A major goal of the project is to arouse fascination and convey the importance of basic research in order to attract the female scientists of tomorrow. In a scientific accompanying study, the mechanisms of the career choice decisions of high school students and the role of social barriers are examined from an interdisciplinary perspective using methods of empirical social research.



References:

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From Science to Start-Up

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A broad range of outstanding research projects are carried out every day at universities in Münster and throughout the EUREGIO area, yet many researchers are unaware of the opportunities that start-ups offer as a potential career path. We have established a special service to address researchers, students and members of Münsters' universities to support them in their ambitions of becoming business founders. The interdisciplinary REACH-Team encourages and aids interested parties via coaching, teaching, with special workshops and structured programs (e.g. for Start-up funding) in order to support upcoming business ideas resulting from intense scientific research and results.

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