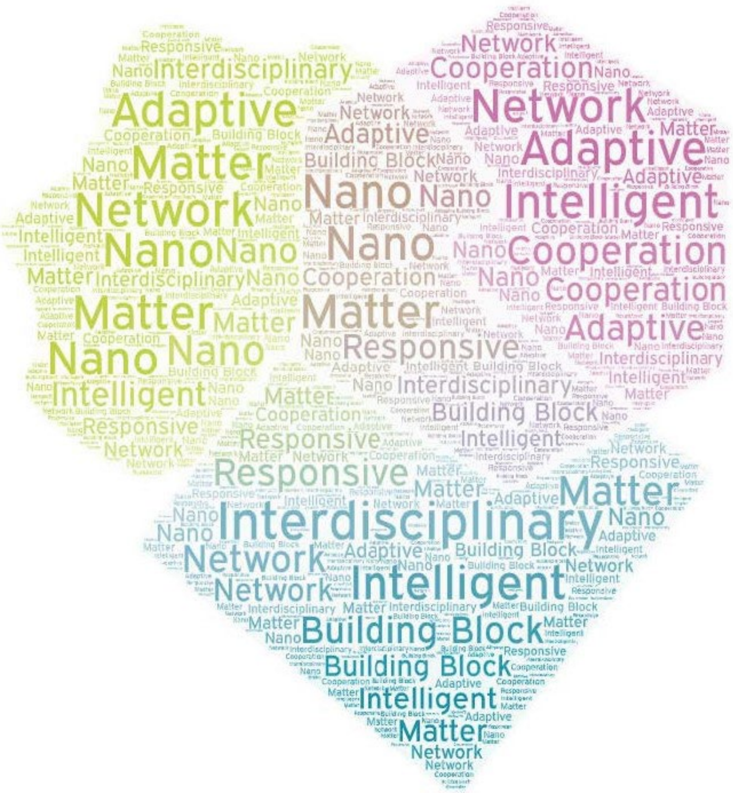
Westfälische
Wilhelms-Universität
Münster

Center for Soft Nanoscience

CRC 1459
INTELLIGENT
MATTER

1st Münster Symposium on Intelligent Matter

22. June 2022
Münster, Germany



Book of Abstracts

MüSIM2022 Speakers

Prof. Dr. Friedrich Simmel

Chair of Physics of Synthetic Biological Systems
Department of Physics
Technical University of Munich
Garching, Germany

The research conducted by Prof. Simmel revolves around bionanotechnology and the physics of synthetic biological systems. His particular areas of interest include artificial molecular machines and nanostructures composed of DNA molecules and the design of artificial biochemical circuits.

After studying physics and completing his doctorate (1999) at Munich's Ludwig Maximilian University (LMU), he did research work at Bell Laboratories in Murray Hill, NJ, USA. He returned to LMU in 2002 to work in a junior research group sponsored by the German Research Foundation's Emmy Noether program. In 2005, Prof. Simmel qualified as a lecturer in experimental physics at LMU. He has been Chair of Experimental Physics (Physics of Synthetic Biological Systems) at TUM since 2007. Since 2013, Prof. Simmel has been a member of acatech - the National Academy of Science and Engineering.

Molecular devices made from DNA

Friedrich Simmel, TU München, GER

Over the past decades, the sequence-controlled interactions between DNA molecules have been used to "program" self-assembly processes that resulted in the realization of ever more complex nanostructures made from DNA.

Integration of other chemistries, molecular recognition elements, simple information-processing capabilities, and also mechanical functions has led to the realization of a wide range of molecular devices, some of which act molecular machines or even nanoscale "robots".

In the talk, a brief overview of DNA nanotechnology will be given, followed by a few examples of DNA nanomachines and robotic systems.

MüSIM2022 Speakers

Prof. Dr. Nathalie Katsonis

Faculty of Science and Engineering, Active Molecular Systems
University of Groningen
Groningen, The Netherlands

Nathalie Katsonis received her MSc (2001) and PhD (2004) degrees from the University Pierre et Marie Curie (Paris, France). Her investigations of the interplay between motion, light and molecular machines started in the group of Ludovic Jullien, where she researched the chromophore that initiates the flagellar movement of purple bacteria. For her postdoctoral research she moved to the group of Ben Feringa to investigate chirality and order in supramolecular assemblies.

Her independent career started in 2007 as Associate Researcher for the French National Center for Scientific Research. In 2008 she was invited back to Groningen to work with Feringa on artificial molecular motors and switches. In 2011 she took up a tenure-track position at the MESA+ Institute for Nanotechnology at the University of Twente (the Netherlands), where she was promoted to Associate Professor in 2014 and to Full Professor in 'Bio-inspired and Smart Materials' since 2017. In March 2020 she joined the Stratingh Institute of Chemistry of the University of Groningen (the Netherlands), as Professor of 'Active Molecular Systems and Materials'.

Katsonis has led the way in transmitting directed molecular motion across length scales, with a special focus on the role of chirality and on the effects of mechanically-relevant motion of molecular machines. Her achievements have provided the underpinnings for increasingly complex functionalities in dynamic and ultimately life-like supramolecular materials.

Chemical systems in motion

Nathalie Katsonis, Stratingh Institute for Chemistry, University of Groningen, NL

Motion is a hallmark of life and is born from the chemistry of interacting molecules. My research group is concerned with discovering the molecular systems and mechanisms at the origin of movement, both in time and in space, from the nanoscale upwards [1]. Unravelling the rules of molecular motion is likely to have profound consequences in understanding the world around us. Moreover, re-engineering motion from the molecular scale upwards is also a means to achieve unconventional functionalities in life-like, adaptive and, ultimately, intelligent materials [2].

Over the past 15 years, I have focused my research on three fundamental challenges: deciphering the mechanics of individual molecules, coupling mechanically active molecular processes with the molecules surrounding them as to achieve macroscopic responses, and transducing macroscopic motion into motility. Here, I will present some of our recent work on the design and synthesis of motile chemical systems [3]. In particular, I will show examples in which motile droplets evolve intelligent behaviour in lipid systems, including mutualism between chemistry and motion, light-responsiveness, chemotaxis, and photokinesis.

1. A. Aspuru-Guzik, et al, *Nature Chemistry* 2019, 11, 286 – 294.
2. F. Lancia, A. Ryabchun, N. Katsonis, *Nature Reviews Chemistry* 2019, 3, 536–551.
3. D. Babu, N. Katsonis, F. Lancia, R. Plamont, A. Ryabchun, *Nature Reviews Chemistry* 2022, https://doi.org/10.1038/s41570-022-00392-8

MüSIM2022 Speakers

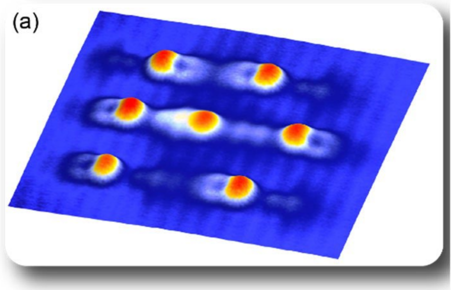
Prof. Dr. Alex Khajetoorians

Institute of Molecules and Materials
Scanning Probe Microscopy Department
Radboud University
Nijmegen, The Netherlands

Alexander Ako Khajetoorians has been full professor and head of the SPM department, at the Institute for Molecules and Materials, since fall 2014. His research focuses on characterizing and manipulating the electronic and magnetic properties of quantum materials at the scale of a single atom. Utilizing scanning probe microscopy, he has helped advance numerous spin-resolved methods. He has established one of the most advanced and high precision laboratories in the world at Radboud University, with the highest resolution microscope in the Netherlands, dedicated toward understanding and ultimately utilizing the novel properties of new materials for energy-efficient information technology and sensing. He has been awarded prestigious personal grants, such as an Emmy Noether group (DFG) in 2013, a VIDI grant (NWO) in 2015, and an ERC Consolidator Grant in 2018 (SPINAPSE). Prof. Khajetoorians has also been awarded the Gerhard Ertl Young Investigator Award in 2012, and the Nicholas Kurti European Prize in 2014.

What can we 'learn' from atoms? going beyond neuromorphics

Alex Khajetoorians, Scanning probe microscopy department, Institute for Molecules and Materials
Radboud University, NL



The quest to implement machine learning algorithms in hardware has focused on combining various materials, each mimicking a computational primitive, to create device functionality. These endeavors have led to the beautiful development of dedicated hardware that, working in combination with software, can perform pattern recognition tasks. Ultimately, these piecewise approaches limit functionality and efficiency, while complicating scaling and on-chip learning, necessitating new approaches linking physical phenomena to machine learning models. Likewise, this raises the question if there are new machine learning algorithms to be discovered, utilizing the particular properties of quantum properties of matter where there are no obvious links to established models. Here, I will discuss the first steps toward a new paradigm in computing, routed in fundamentals studies based on the idea of letting the physics do the work. I will introduce the concept of an atomic orbital memory and how coupling leads to tunable multi-well landscapes. I will discuss how the ensuing stochastic dynamics mimics the perennial model in machine learning, the Boltzmann machine. In this discussion, I will review the emergence of multiple and separable time scales, an adaption of long-term potentiation in biological matter, which serves the basis for self-adaption. I will also discuss more recent develops moving toward local gate control of stochastic behavior, AC response, and finally new types of orbital memory. I will conclude with an outlook on concepts that go beyond the current neuromorphic paradigm, combining concepts related to quantum coherent and quantum technologies.

MüSIM2022 Speakers

Prof. Dr. Dirk Englund

Institute for Soldier Nanotechnologies

Electrical Engineering and Computer Science Section
Massachusetts Institute of Technology
Cambridge, MA, USA

Dirk Englund received his BS in Physics from Caltech in 2002. After a Fulbright fellowship at T.U. Eindhoven, he completed an MS in Electrical Engineering and a PhD in Applied Physics at Stanford University in 2008. After a postdoctoral fellowship at Harvard University, he joined Columbia University as Assistant Professor of Electrical Engineering and of Applied Physics. In 2013, he joined the faculty of MIT's Department of Electrical Engineering and Computer Science. Major recognitions include the 2011 Presidential Early Career Award in Science and Engineering, the 2011 Sloan Fellowship in Physics, the 2012 DARPA Young Faculty Award, the 2012 IBM Faculty Award, a 2016 R&D100 Award, the OSA's 2017 Adolph Lomb Medal, the 2017 ACS Photonics Young Investigator Award, the Bose Research and the Humboldt Research Fellowships. He’s a fellow of Optica. Further, he was involved in the startups Dust Identity (co-founder), LightMatter (advisor), and QuEra Computing (co-founder).

Error-correction in electro-optic accelerators for machine learning

Dirk Englund, Research Laboratory of Electronics & Dept of EECS, MIT, USA

As deep neural networks (DNNs) are remaking machine learning, critical hardware challenges are emerging in various aspects of existing conventional electronics, including throughput and energy consumption. This has motivated a search for new hardware architectures optimized for artificial intelligence, such as electronic systolic arrays, memristor crossbar arrays, and optical accelerators. Optics can perform linear matrix operations at exceptionally high rate and efficiency, motivating recent demonstrations of low latency linear algebra and energy consumption that is below a single photon per multiply-and-accumulate operation. However, a central challenge is to model and experimentally test full systems, so that we can understand scaling of performance metrics including the above-mentioned throughput, energy consumption, but critically also error rate and its dependence on hardware imperfections. This talk will consider these questions on various weight-stationary and output-stationary hardware platforms, with a particular focus on recently discovered hardware error correction methods and in-situ training methods.

MüSIM2022 Young Researcher Awardee

Mehak Jain, M.Sc.

Organic Chemistry Institute
University of Münster
Münster, Germany

For her contribution

Fuel-Driven and Enzyme-Regulated Redox-Responsive Supramolecular Hydrogels
Mehak Jain and Bart Jan Ravoo
Angew. Chem. Int. Ed. **2021**, 60, 2 1062–21068

Chemical reaction networks (CRN) embedded in hydrogels can transform responsive materials into complex self-regulating materials that generate feedback to counter the effect of external stimuli. This study presents hydrogels containing the β-cyclodextrin (CD) and ferrocene (Fc) host–guest pair as supramolecular crosslinks where redox-responsive behavior is driven by the enzyme–fuel couples horse radish peroxidase (HRP)–H_2O_2 and glucose oxidase (GO_x)–D-glucose. The hydrogel can be tuned from a responsive to a s elf-regulating supramolecular system by varying the con-centration of added reduction fuel D-glucose. The onset of self-regulating behavior is due to formation of oxidation fuel in the hydrogel by a cofactor intermediate GO_x[FADH2]. UV/Vis spectroscopy, rheology, and kinetic modeling were employed to understand the emergence of out-of-equilibrium behavior and reveal the programmable negative feedback response of the hydrogel, including the adaptation of its elastic modulus and its potential as a glucose sensor.

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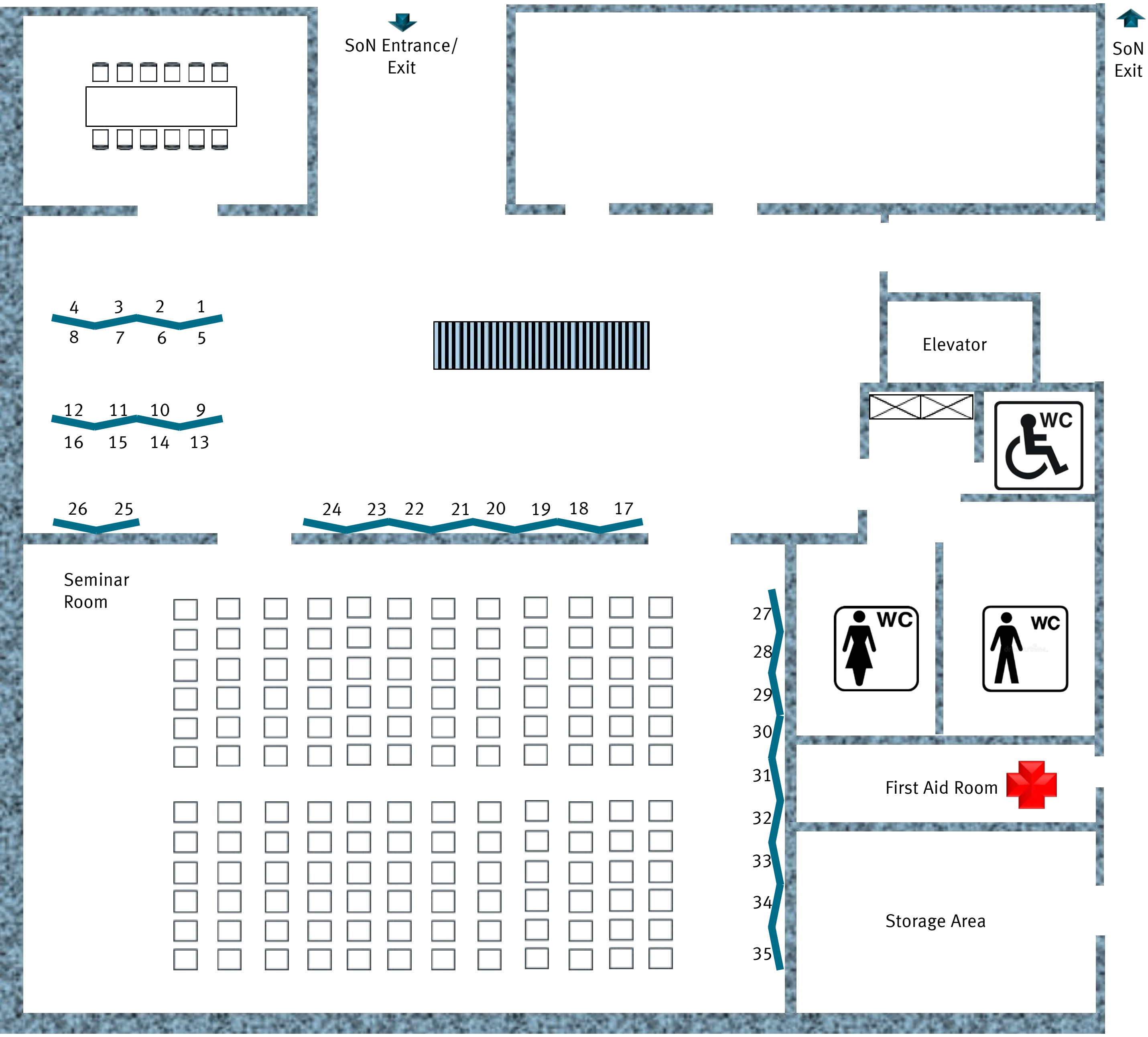
Poster Sessions Setup



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

MüSIM2022 Poster Contributions

(alphabetical order first author´s surname))

01. Beyond workfunctions: the influence of substrate on intermolecular interactions of 11-MHQ
Fuad A. Alami and Christian A. Nijhuis
University of Twente

02. Deep neural networks with photonic activation functions
Marlon Becker, Jan Riegelmeyer, Alexander Eich, Maximilian Seyfried, B.J. Ravoo, Carsten Schuck, Benjamin Risse
University of Münster

03. Combining electrodynamics, light and memory to create intelligent in-materio computing devices
Ivonne Bente[1], Lorenzo Cassola[1,2], Reinier Cool[1,2], Thomas Grottke[1], Wilfred G. van der Wiel[1,2], Wolfram Pernice[1]
[1] University of Münster, [2]University of Twente

04. Self-assembly of hybrid nanostructures for brain-inspired electronics
Marc Beuel[1,2], Jonas Mensing[2], Lisa Schlichter[2], Hidde Veldkamp[1], Andreas Heuer[2], Bart Jan Ravoo[2], Wilfred van der Wiel[1,2]
[1]University of Twente, [2]University of Münster

05. Philosophical aspects of intelligent matter
Antonio Bikic
University of Münster, TU Munich

06. Peptides with specific binding activities to crystals for diagnosis of gout and pseudogout
Ji-Hong Bong[1,2], Jae-yong Jung[2], Jae-Chul Pyun[2], and Joachim Jose
[1]University of Münster, [2]Yonsei University

07. Novel dynamic molecular switches based on HATNA derivatives
Alessandro Borrini, Saurabh Soni, Fuad A. Alami and Christian A. Nijhuis
University of Twente

08. Photoswitches for integration in adaptive Nanosystems
Florian Bosse, Mowpriya Das, Malte Schrader, Ashutosh Kanojiya, Lisa Schlichter, Frank Glorius, Bart Jan Ravoo
University of Münster

09. Electron microscopy studies on *S. cerevisiae* peroxisomal import machinery utilizing synthetic cargo
Cole Bourque[1,2] and Maximillian Rüttermann[1], Pascal Lill[1,2], Benedikt Pascal Nowak[1], Luca Burg[1], Tomasz Jeziorek[3], Tobias Hansen[3], Ralf Erdmann[3], Bart Jan Ravoo[1], Christos Gatsogiannis[1,2]
[1]University of Münster, [2]Max Planck Institute of Molecular Physiology Dortmund, [3]Ruhr University Bochum

MüSIM2022 Poster Contributions

(alphabetical order first author´s surname))

10. **Reservoir computing in human movement science**
Myriam Lauren de Graaf, Luis Mochizuki, Frederik Thies, Heiko Wagner, and Charlotte Le Mouel
University of Münster

11. **Linear and nonlinear propagation of short spin-wave pulses in microscopic YIG waveguides**
Boris Divinskiy[1], Hugo Merbouche[1], Kirill O. Nikolaev[1], Jannis Bensmann[1], Paul Steeger[1], Johann A. Preuß[1], Robert Schmidt[1], Robert Schneider[1], Johannes Kern[1], Steffen Michaelis de Vasconcellos[1], Dmitrii Raskhodchikov[1], Corinna Kaspar[1], Diane Gouéré[2], Romain Lebrun[2], Vincent Cros[2], Jamal Ben Youssef[3], Paolo Bortolotti[2], Abdelmadjid Anane[2], Vladislav E. Demidov[1], Rudolf Bratschitsch[1], Sergej O. Demokritov[1], Wolfram H. P. Pernice[1]
[1] University of Münster, [2]Université Paris-Saclay, [3]Université de Bretagne Occidentale LabSTICC

12. **Interfacing self-assembly and multiple stimuli to create adaptive behavior**
Torsten Dünnebacke, Niklas Niemeyer, Sebastian Hochstädt, Gustavo Fernandez, Michael Ryan Hansen, Johannes Neugebauer
University of Münster

13. **Synthesis of polymers bearing a chiral backbone via stereospecific ionic ring-opening polymerization of chiral donor-acceptor cyclopropanes and Alternating Terpolymers through Cyclopolymerization and Subsequent Orthogonal Functionalization**
Alexis Emmerich, Constantin G. Daniliuc, Philipp Gerdt, Armido Studer
University of Münster

14. **Design of chemoenzymatic toolboxes for orthogonal biomolecular labeling**
Mehmet Erguven, Nicolas V. Cornelissen, Aileen Peters, Ann-Marie Lawrence, Ezgi Karaca, Andrea Rentmeister
University of Münster

15. **Control and responsiveness of air-water interfaces with photoswitchable arylazopyrazole surfactants**
Michael Hardt[1], Franziska Busse[1], Christian Honnigfort[1], Javier Carrascosa- Tejedor[2,3], Philipp Gutfreund[2], Richard A. Campbell[3], Andreas Heuer[1] and Björn Braunschweig[1]
[1]University of Münster, [2]Institut Laue-Langevin, [3]University of Manchester

16. **History-dependent signal processing in a flow reactor**
Dmitrii V. Kriukov and Wong Asy
University of Twente

17. **Single-walled carbon nanotubes as near-infrared fluorescent biosensors**
Justus T. Metternich[1,2], Julia Ackermann[1,2], Svenja Herbertz[1,2] and Sebastian Kruss[1,2]
[1]Fraunhofer Institute of Microelectronic Circuts and Systems, [2]Ruhr-University Bochum

MüSIM2022 Poster Contributions

(alphabetical order first author´s surname))

18. Chirality-induced electron spin polarization in chiral CuO and CoOx catalyst surfaces
Paul V. Möllers[1], Jimeng Wei[2], Supriya Ghosh[2], Soma Salamon[3], Manfred Bartsch[1], Heiko Wende[3], David H. Waldeck[2], Helmut Zacharias[1]
[1]University of Münster, [2]University of Pittsburgh, [3]Universität Duisburg-Essen

19. Adaptive cell-matrix Nanosystems
Theresa Mößer[1], Tobias Rex[1], Inka Schröter[2], Tobias Theiss[1] , Carsten Grashoff[1], Cristian A. Strassert[1] and Britta Trappmann[2]
[1]University of Münster, [2]MPI Molecular Biomedicine

20. H-bonded ambipolar supramolecules for room temperature ferroelectricity
Anurag Mukherjee,[1] Shubhankar Barman[2], Anupam Ghosh[2], Saptarshi Chakraborty[2], Anuja Datta[2] and Suhrit Ghosh[2]
[1]University of Münster, [2]Indian Association for the Cultivation of Science

21. Developing tunable triplet emitters towards adaptive electroluminescent materials
Helena Osthues, Stefan Buss, Cristian A. Strassert, Nikos L. Doltsinis
University of Münster

22. Programmable control of gene expression using non-natural AdoMet analogs
Aileen Peters, Raminta Mineikaitė, Anna-Maria Böttick, Jonas Schöning and Prof. Dr. Andrea Rentmeister
University of Münster

23. Ultra-fast dynamics in thiophene-based conjugated donor-acceptor organic polymers
Tobias Reiker[1], Carsten Winter[1], Deb Kumar Bhowmick[1], Nils Fabian Kleimeier[1], Zitong Liu[2], Deqing Zhang[2] and Helmut Zacharias[1]
[1]University of Münster, [2]Chinese Academy of Science

24. Smart Matters 4 You
Julian Repke
University of Münster

25. Emissive alcohol low-molecular-weight gelators (LMWGs)
Kevin Rudolph, Jens Voskuhl
University of Duisburg-Essen

26. Towards intelligent light-propelled nano- and microsystems
Matthias Rüschenbaum, Julian Jeggle, Cornelia Denz, Raphael Wittkowski
University of Münster

MüSIM2022 Poster Contributions

(alphabetical order first author´s surname))

27. **Breakdown of dipolar blueshift at low-temperatures indicating quantum correlations in exciton ensembles in WSe2-MoSe2 hetero-bilayer**
    Nihit Saigal[1], Torsten Stiehm[1], Hendrik Lambers[1], Florian Sigger[2], Lukas Sigl[2], Mirco Troue[2], Johannes Figueiredo[2], K. Watanabe[3], T. Taniguchi[3], Alexander W. Holleitner[2] and Ursula Wurstbauer[1]
    [1] University of Münster, [2]TU Munich, [3]National Institute for Materials Science Japan

28. **Photoinduced synthesis of luminescent dibenzothiophenes in polymer matrices**
    Marco Schmiedtchen, Jens Voskuhl
    University of Duisburg-Essen

29. **Dual-functional memory behavior in EGaIn-PEDOTPSS-Au devices**
    Saurabh Soni, Fuad A. Alami, and Christian A. Nijhuis
    University of Twente

30. **Light-controlled anion binding supramolecular-systems**
    Pascal Steinforth[1], Leon Hoppmann[2], Lukas Entgelmeier[2] Leonard Wyszinski[1], Olga García Mancheño[2], Monika Schönhoff[1]
    University of Münster

31. **Exciton species in highly doped WS_2 monolayers**
    David O. Tiede, Hendrik Lambers, Hossein Ostovar, Nihit Saigal, Ursula Wurstbauer
    University of Münster

32. **Mixed-mode in-memory computing using adaptive phase-change materials**
    Niklas Vollmar, Daniel Wendland, Akhil Varri, Wolfram Pernice, Martin Salinga
    University of Münster

33. **From science to start-up**
    Anne Vortkamp
    Reach Euregio Start-Up Center

34. **Photolithography with green to far-red light for protein micro patterns**
    Yanjun Zheng, Fei Chen, and Seraphine Wegner
    University of Münster

35. **Adaptive polymer morphologies through reversible block fragmentation**
    Katharina Ziegler[1], Yorick Post, André Gröschel and Bart Jan Ravoo
    University of Münster

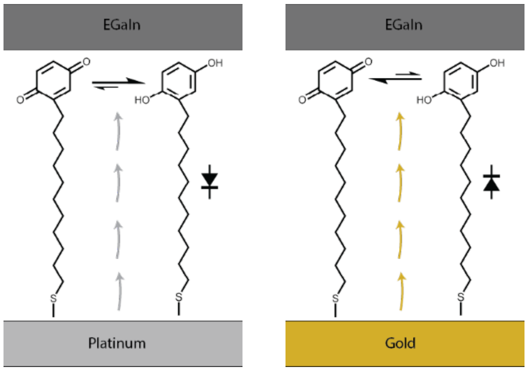
MüSIM2022 Poster Abstracts

1

Beyond workfunctions: the influence of substrate on intermolecular interactions of 11-MHQ

Fuad A. Alami and Christian A. Nijhuis

University of Twente, Hybrid Materials for Optoelectronics
Drienerlolaan 5, 7522 NB, Enschede, The Netherlands
f.a.alami@utwente.nl



Intelligent design of energy level alignment for molecular electronics is crucial for developing complex charge transfer systems. The majority of approaches for energy level alignment pertain to chemical modification. However, molecule-electrode interactions can also present a means of modulating alignment within the junction via interactions such as push-back effects[1] and Fermi level pinning[2]. In addition, substrate-mediated interactions can induce structural, chemical, and electronic changes in self-assembled monolayers.[3] To the best of our knowledge, studies between the coupling of a proton-coupled electron transfer (PCET) system and substrate-mediated interactions have yet to be investigated. In these studies, we study the influence of substrate choice on the well-known PCET demonstrated in hydroquinone redox reactions. By using 11-mercaptoundecylhydroquinoine (11-MHQ) tethered to platinum or gold, we can differentiate the substrate's influence on the charge transfer mechanism. We investigated whether the substrate influences the redox equilibrium by characterizing the monolayer by Fourier transform infrared spectroscopy (FTIR) and cyclic voltammetry (CV). Furthermore, a manifestation of such influences is demonstrated by forming a two-terminal junction composed of metal/11-MHQ/EGaIn (eutectic alloy of gallium and indium). These junctions demonstrated a reversal in rectification only dependent on electrode choice.

1. Heimel, Georg, et al. *Accounts of Chemical Research*, vol. 41, no. 6, 2008, pp. 721–729., https://doi.org/10.1021/ar700284q.
2. Amsalem, P., et al. *Physical Review B*, vol. 87, no. 3, 2013, https://doi.org/10.1103/physrevb.87.035440.
3. Sykes, E. Charles, et al. "Substrate-Mediated Interactions and Intermolecular Forces between Molecules Adsorbed on Surfaces." *Accounts of Chemical Research*, vol. 36, no. 12, 2003, pp. 945–953., https://doi.org/10.1021/ar970286l.

2

Deep neural networks with photonic activation functions

Marlon Becker[1], Jan Riegelmeyer[2], Alexander Eich[2], Maximilian Seyfried[3], B.J. Ravoo[3], Carsten Schuck[2], Benjamin Risse[1]

[1] *University of Münster, Institute for Computer Science and Institute for Geoinformatics, 48149 Münster, Germany*
[2] *University of Münster, Institute of Physics and Center for NanoTechnology, 48149 Münster, Germany*
[3] *University of Münster, Institute of Organic Chemistry, 48149 Münster, Germany*
marlonbecker@uni-muenster.de

Optical artificial neural networks (OANNs) with coherent nanophotonic circuits hold the potential of fast and energy efficient information processing. However, the implementation of nonlinear nanophotonic components, required to implement the nonlinear character necessary for artificial neural networks (ANNs) in the form of activation functions, remains a major challenge. We utilize the nonlinear photoswitching behavior of azobenzenes to train deep neural networks. Therefore, we characterize the absorption of an azobenzene solution in a free space experiment. In particular, 468 nm irradiation wavelength is used to induce a nonlinear absorption in an information carrying signal of 532 nm. An analytical function comprising a linear and nonlinear part is fitted to the absorption curve while the experimental noise is modeled by a Gauss distribution. This function is subsequently used as a nonlinear activation function to train neural networks on well-known image classification benchmarks such as the handwritten numbers dataset MNIST. By changing the coefficients of our activation function we can tune the amount of nonlinearity within the underlying optimization task and analyze the resulting classification performance. Interestingly our results indicate the existence of certain lower and upper bounds of nonlinearity. In fact, we were able to identify a sufficient strength of nonlinearity to achieve significant performance advancements in all our experiments, which feed back into the chemical and physical design of the experimental setup. We therefore conclude that azobenzene solutions can be used to develop nonlinear building blocks for OANNs.

3

Combining electrodynamics, light and memory to create intelligent in-materio computing devices

Ivonne Bente[1,2,3,*], Lorenzo Cassola[1,4,5], Reinier Cool[1,4,5], Thomas Grottke[1,2,3], Wilfred G. van der Wiel[1,4,5] and Wolfram H.P. Pernice[1,2,3]

[1] *University of Münster, Center for Soft Nanoscience (SoN),*
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[2] *Physikalisches Institut, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany*
[3] *CeNTech – Center for Nanotechnology, Heisenbergstr. 11, 48149 Münster, Germany*
[4] *University of Twente, Faculty of Electrical Engineering, Mathematics and Computer Science,*
Hallenweg 23, 7522NH, Enschede, The Netherlands
[5] *BRAINS Center for Brain-Inspired Nano Systems and MESA+ Institute for Nanotechnology,*
University of Twente, Drienerlolaan 5, 7522 NB Enschede, The Netherlands
[*] *i.bente@uni-muenster.de*

As members of the C02 project, our main ambition is to develop devices for neuromorphic architectures, but, in order to achieve this goal, we are moving in different directions and exploring various possible solutions. On the one hand, we are focusing on in-materio computation, trying to develop smart, energy-efficient devices, which, thanks to their internal complexity and transport properties, have highly nonlinear behaviour. For this purpose, we are currently studying silicon-based, tunable processing units and light-activated perovskites. This would allow us to have building blocks for in-hardware electrical neural networks, that are able to perform complex classification tasks. At the same time, we are also working on photonic integrated circuits for tunable and reconfigurable optical networks, which are essential for optical neu-ral networks and photonic memory computing. Regarding this area of interest, we established nanofabrication of plasmonic nanoantennas and opto-mechanical phase shifters, both enabling highly efficient refractive index tuning. This feature makes them optimal candidates for being used as computational nodes in optical neuromorphic architectures. Moreover, all these technologies could in principle be combined with phase change materials to obtain memory functionality, reproducing not only neurons' features, but also a synaptic-like behaviour.

4

Self-assembly of hybrid nanostructures for brain-inspired electronics

Marc Beuel[1,2,3,4], Jonas Mensing[5], Lisa Schlichter[3], Hidde Veldkamp[1], Andreas Heuer[5], Bart Jan Ravoo[3], 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, Westfälische Wilhelms-Universität, Busso-Peus-Straße 10, 48149 Münster, Germany*
[4]*Physikalisches Institut, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany*
[5]*Institut für Physikalische Chemie, Westfälische Wilhelms-Universität, Corrensstraße 28-30, 48149 Münster, Germany*
marc.beuel@uni-muenster.de

We want to achieve reconfigurable computational functionality in a *designless* nanoparticle network for machine learning applications using artificial evolution in nanoscale materials. Previous research[1] 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.

1. S. K. Bose, C. P. Lawrence, Z. Liu, K. S. Makarenko, R. M. J. van Damme, H. J. Broersma, W. G. van der Wiel, *Nat. Nanotechnol.* **2015**, *10*, 1048–1052.

5

Philosophical aspects of intelligent matter

Antonio Bikić

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»Intelligent matter« represents a very promising approach from a philosophical point of view, which, on the one hand, can test functionalism. On the other hand, and motivated by Moravec's paradox, intelligent matter can also be used to outline what an epistemic approach to the world that is grounded in realism must look like.

This paper explores the nature of teleonomic processes with a special focus on the question if these processes can be realized in »intelligent matter«. The scientific problem it tackles arises from the question whether teleonomic processes are strictly limited to »living matter«. If it is indeed possible to make way for artificially generated teleonomic processes, »intelligent matter« might benefit from this, among others, in terms of responsiveness.

The primary research question is the following: is it possible to generate teleonomic processes out of »intelligent matter«? This paper answers this question by shedding light on the connection between *abstract* and *concrete* computation. The thesis is: if a functionalist realization of teleonomic processes is in fact possible, all memory structures can only be *mnemoid structures* due to them not being cognized. Mnemoid structures, as they occur e.g. in slime molds (*physarum polycephalum*), do not save memories in the same way cognitive systems do. This is why remembering things *without cognition* leads to different behavior. One of the goals of this paper is therefore to determine the difference between these two types of knowledge storage and knowledge generation.

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Peptides with specific binding activities to crystals for diagnosis of gout and pseudogout

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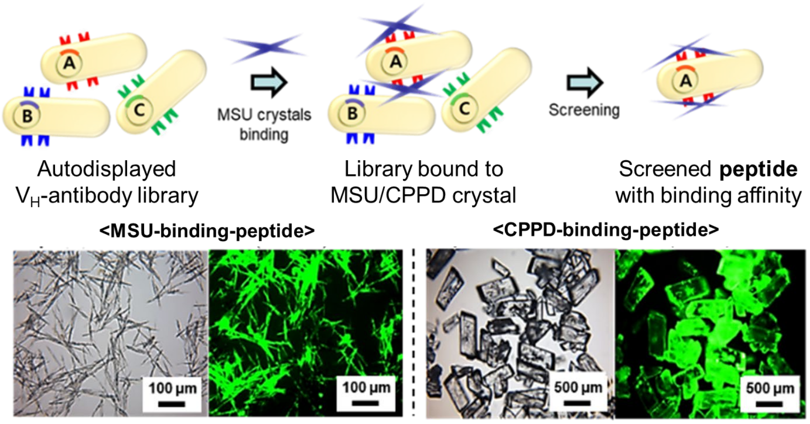

To date, medical diagnosis of gout and pseudogout has been performed by observing the crystals in the joint fluid of patients under a polarized microscope. Conventional diagnostic methods using a polarized microscope have disadvantages, such as time-consuming analysis, a high false negative rate, and difficulty in distinguishing gout with monosodium urate (MSU) crystals and pseudogout with calcium pyrophosphate dihydrate (CPPD) crystals in synovial fluids. In this study, a chromogenic assay for the diagnosis of gout and pseudogout, without the requirement of a polarized microscope and trained experts, was proposed using peptides with specific binding activities to MSU and CPPD crystals. The V_H-antibody library with randomized complementarity-determining region 3 (CDR3) region was expressed on the outer membrane of *Escherichia coli* using autodisplay technology. The target antibodies with binding activity to MSU and CPPD crystals were screened from the library, and five clones were selected. The peptides originated from the CDR3 sequences of the selected clone were chemically synthesized. The binding properties of the synthetic peptides were analyzed using fluorescence imaging and flow cytometry, and the affinity constants (K_D) against MSU and CPPD crystals. A chromogenic assay configuration for gout and pseudogout was developed using the synthetic peptides. In this chromogenic assay, synthetic peptides labeled with biotin and streptavidin– horseradish peroxidase(HRP) complex were used, and crystal detection was possible using a chromogenic reaction between HRP and a chromogenic substrate (TMB). Finally, gout and pseudogout were diagnosed by detecting MSU and CPPD crystals in the synovial fluid in the concentration range of 0–300 µg/mL.

Novel dynamic molecular switches based on HATNA derivatives

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Synaptic plasticity is an essential requirement for materials trying to emulate human brain operations. Currently, most approaches to neuromorphic computing rely on high energy consuming silicon materials.[1] An attractive energy efficient solution is given by molecular switches which can emulate 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 Ca^{2+} 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.[2] Synthetic modification of HATNA with diphenylacetylene (DPA) moieties can potentially facilitate charge transport through the molecule while at the same time enhance packing density of molecules on the electrode.[3,4] In this poster we give an overview of the synthesis route to achieve the dynamic switch HATNA-DPA.

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8

Photoswitches for integration in adaptive nanosystems

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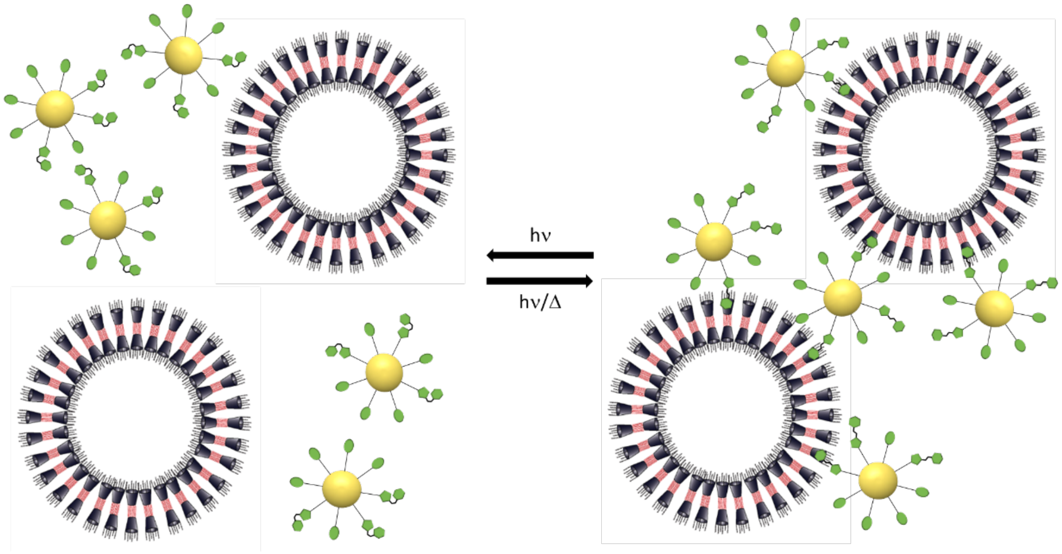
In the development of intelligent matter, photoresponsive materials can act as an important building block to realize the four key functional elements: sensor, actuator, network and long-term memory.[1] Therefore, we present gold nanoparticles functionalized with a mixed ligand shell containing arylazopyrazoles (AAPs) as photoresponsive unit. In doing so, the advantages of AAPs as excellent photoswitches and the surface plasmon of the particles can be combined in a single material.

In a first part of the project, thiolated AAP was employed as a responsive ligand in combination with a dummy ligand, in order to sustain responsiveness and tune solubility.[2,3] Subsequently, the photophysical properties of the obtained particles were analyzed and the particles were deployed as linker for cyclodextrin vesicles.

In a second part of the project, new photoswitches conjugated with N-heterocyclic carbenes (NHCs) have been developed. In previous studies, NHCs have proven to be a superior gold ligand compared to thiols.[4] Therefore, we intend to deploy these new photoswitches as novel ligands in gold surface and nanoparticle applications.



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9

Electron microscopy studies on *S. cerevisiae* peroxisomal import machinery utilizing synthetic cargo

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Peroxisomes are crucial organelles involved in redox balance and detoxification in eukaryotic cells. Interestingly, these organelles import native and even oligomerized proteins from the cytosol via transient import channels, as they lack genetic information and ribosomes. However, formation of these channels is not yet mechanistically understood. Additional knowledge on this topic is urgently needed, as peroxisomes have been shown to be involved in age-related diseases including cancer and diabetes.

It is known that proteins containing one of the three Peroxisomal Targeting Signal (PTS) sequences are transported to the peroxisomal membrane by cytosolic receptors. Cargo-carrying receptors interact with the peroxisomal docking complex followed by import channel formation, cargo import, and finally recycling of the cytosolic receptors. To study this, we have designed a synthetic cargo with an attached PTS sequence to visualize import events using negative stain and cryogenic electron microscopy.

10

Reservoir computing in human movement science

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Animals display rich and coordinated motor patterns during locomotion. Previous modeling and experimental results suggest that the balance between excitation and inhibition in neural networks may be critical for generating such structured motor patterns. However, biological neural networks have an anatomical imbalance between excitatory and inhibitory neural populations.

We explore the influence of anatomical imbalance on the ability of a reservoir computing artificial neural network to learn human locomotor patterns for slow walking, fast walking, and running. We varied the number of neurons, connection percentages, and connection strengths of the excitatory and inhibitory populations.

We showed that performance depended on the network anatomy. First, it deteriorated when the total number of neurons was too small or the total connection strength was too large. Second, performance was critically dependent on the balance between excitation and inhibition. Imbalance towards excitation caused a reduction in the richness of internal network dynamics, leading to a stereotypical motor output and poor overall performance. In contrast, rich internal dynamics and good overall performance were found when the network anatomy was either balanced or imbalanced towards inhibition. This suggests that motor pattern generation may be robust to increased inhibition but not increased excitation in neural networks.

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Linear and nonlinear propagation of short spin-wave pulses in microscopic YIG waveguides

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We study experimentally the linear and nonlinear propagation of short spin-wave pulses in microscopic waveguides made of nanometer-thick yttrium-iron-garnet films. Such waveguides are the key elements of adaptive magnonic networks.

In the linear propagation regime, dispersion usually leads to a significant broadening of spin-wave pulses. We have found that this undesirable effect can be almost completely suppressed resulting in a dispersionless propagation. This is achieved by using the competing effects of the dipolar and exchange interactions, which can be controlled by changing the waveguide geometry. In the nonlinear regime, we observed an exceptionally strong phase modulation of spin-wave pulses. We have found that this phenomenon causes an extreme broadening of the spectrum of the pulses resulting in a strong spatial variation of the spin-wave wavelength and a temporal variation of the spin-wave phase across the pulse. The experimental findings are in good agreement with the results of micromagnetic simulations and analytical calculations.

On the one hand, our results demonstrate the great potential of magnonic systems for high-speed information processing networks. On the other hand, they emphasize the importance of understanding the complex nonlinear wave processes in microscopic magnetic structures for successful technical applications of spin waves in integrated magnonic devices.

Interfacing self-assembly and multiple stimuli to create adaptive behaviour

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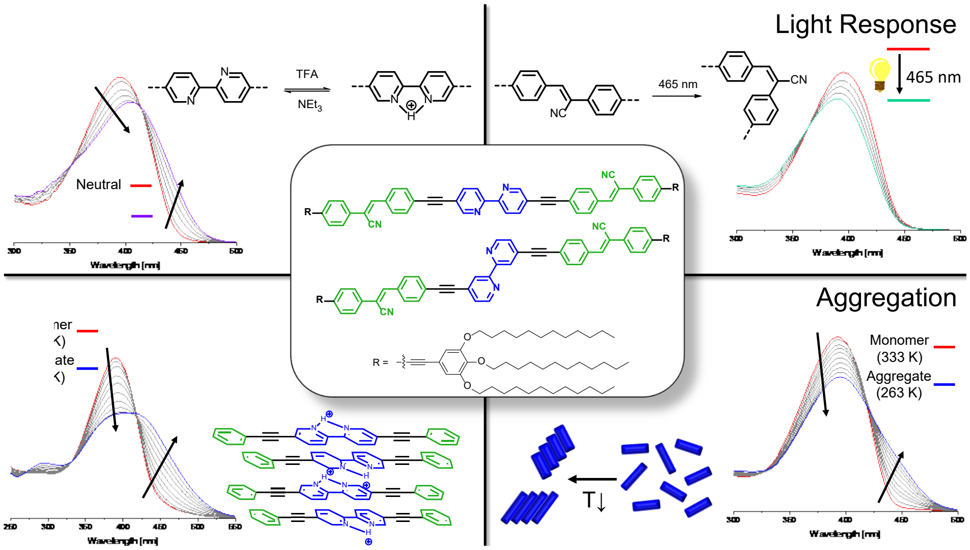
For the targeted development and use of responsive and adaptive nanomaterials, fundamental and mechanistic understanding of the interplay between self-assembly and stimuli-responsive behavior of complex supramolecular systems is indispensable.[1]

To investigate the mutual influence of various separate stimuli on the supramolecular self-assembly, a discrete π-conjugated chromophore with two independent responsive moieties (pH[2] and UV-light[3]) was synthesized. Within this project, understanding and controlling the pathways of the resulting supramolecular assemblies will be the main task of this work. To elucidate the underlying self-assembly mechanisms and the adaptive responses, a variety spectroscopic (UV-vis, Fluorescence, IR) and microscopic (AFM, SEM, DLS) techniques are used. To enable efficient calculations for characterizing the supramolecular structures, theoretical methods are developed that vastly expand the applicability of already 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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13

Synthesis of polymers bearing a chiral backbone via stereospecific ionic ring-opening polymerization of chiral donor-acceptor cyclopropanes

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Many natural processes rely on enantiopure biomacromolecules like DNA and proteins. Thus, the synthesis of chiral unnatural polymers is of increasing interest. The stereospecific ionic ring-opening polymerization of various donor-acceptor cyclopropanes is reported. The chiral cyclopropane monomers are readily prepared and stereospecific polymerization is best conducted with a catalytic amount of MgBr2 serving as a Lewis acid and as an initiator. Polymers with molecular masses of up to 7800 g mol-1 containing a defined 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.
Looking at nature, the defined monomer sequence of biopolymers is mainly responsible for their unique function. However, sequence remains one of the biggest challenges of modern polymer chemistry. With our novel divinyl monomer bearing a linker moiety we were able to prepare alternating terpolymers by utilizing this monomer in the reversible addition-fragmentation chain transfer (RAFT) polymerization in combination with different electron rich monomers. Owing to the structure of the linker we are able to chemically modify these polymers by using different orthogonal postmodification reactions and a small library of functionalized polymers was prepared.

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Design of chemoenzymatic toolboxes for orthogonal biomolecular labeling

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Over the course of the past decade, the field of methyltransferase-(MTase)-based biomolecular labeling has advanced. Chemistry aspect of labeling has become simpler with one-pot chemoenzymatic cascade reactions, in which methionine adenosyltransferase (MAT) and MTase are combined. In this combination, the thermostable MAT (*Mj*MAT) from *Methanocaldococcus jannaschii* has been proven to be advantageous for AdoMet analogue (MTase "fuel") production[1,2]. By combining *Mj*MAT with different MTases, we can modify DNA, mRNA, and small molecules, enabling their photochemistry and click chemistry applications. This yields molecular systems that react to light or chemical stimuli, respectively. Up to now, we have developed such responsive systems *in vitro* (Figure). However, this causes a separation of the method into *in vitro* and later *in vivo* steps, hindering the flexibility and integrity. For our ultimate goal of developing our responsive systems into adaptive[3] systems, we aim to deploy the labeling strategy directly *in vivo*. To this end, our greatest challenge is the MTase promiscuity, potentially causing background labeling activity in cells[4,5]. In the present study, our ligand engineering has unveiled a set of AdoMet modifications that helped us achieve unique enzyme-ligand complementarity, improving the orthogonality of our model systems.

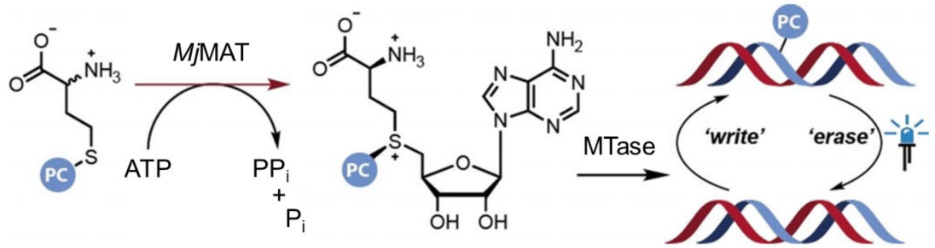

Figure: Photocaging (PC) of DNA in MAT-MTase cascade[1].

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15

Control and responsiveness of air-water interfaces with photoswitchable arylazopyrazole surfactants

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Interfaces that can be changed with different stimuli are of great interest for the development of adaptive materials. One example is the use of alkyl-arylazopyrazole sulfonates (CnAAPC4S) that can undergo *E/Z* photoisomerization. Butyl- AAPC4S surfactants show large photoinduced surface tension (γ) changes at air- water interfaces, which are attributed to massive structural changes at the interface [1].

In order to address these remarkable property changes, we have synthesized two new CnAAPC4S surfactants with an octyl chain or simply hydrogen replacing the former butyl chain. Surface tensiometry reveals that the alkyl tail influences the surface activity drastically, as expected, but also the surfactant's ability to change γ through light irradiation depends strongly on the alkyl tail. The highest surface tension changes are observed for the C4AAPC4S (Δγ~27 mN/m), which is reduced to ~20 or even ‹10 mN/m for octyl and H residues. Using vibrational sum- frequency generation and neutron reflectometry, we provide molecular-level information of the air-water-interface like interfacial composition or the molecular order of the surfactants. Ultra-coarse-grained simulations complement experimental results where the individual surfactant properties like its surface activity or intermolecular interactions can be adjusted to closely reflect the experimental situations and provide information on orientational and structural changes with surfactant concentration.

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16

History-dependent signal processing in a flow reactor

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Multimodal processing of chemical signals is an inherent part of the living matter's adaptation to its environment. The processing significantly relies on history-dependent biochemical circuits that change their state dynamically according to perturbation type, mode, and intensity. Living systems carry processed information in chemicals to trigger dynamic switching events in their internal chemical networks.[1]

Using simple, cost-effective chemicals, a 3D printer, and low-pressure pumps, we designed an autocatalytic network capable of hysteresis and adaptive response to a time-dependent external signal. The network consists of trypsinogen (fuel), trypsin (catalyst) and trypsin inhibitor (inhibitor) in a continuously stirred flow reactor. We demonstrated that the network could exist in two distinct steady states and display a continuum of history-dependent transient states under out-of-equilibrium conditions.[2] We further introduced control over autocatalysis velocity by replacing the trypsin cofactor, making classical binary logic operations such as AND, OR, and XOR possible.

Our study explores the possibility of natural decision making in an elementary biochemical loop. It broadens a conceptual ground for adaptive logic constructions in out-of-equilibrium systems, widely used in a modern neuromorphic matter study.[3]

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17

Single-walled carbon nanotubes as near-infrared fluorescent biosensors

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Biosensors have become powerful tools with important applications in biomedical diagnostics and fundamental research. Especially sensors with an optical readout such as fluorescence offer opportunities for fast, contactless sensing of analytes with high spatial and temporal resolution.

A readout in the near infrared (NIR) is beneficial because of the reduced scattering, autofluorescence and light absorption of biological samples in this spectral range (800 nm – 1700 nm). In this contex, semiconducting single-walled carbon nanotubes (SWCNTs) have emerged as versatile, non-bleaching, NIR-emitting fluorophores. They can be chemically designed in such a way that they specifically interact with biomolecules. This interaction alters the organic phase (corona) around the SWCNT, which modulates their fluorescence.

Here, we present a generic chemical design strategy of DNA-based SWCNT biosensors together with insights into molecular recognition and signal transduction. We showcase the potential of SWCNT-based biosensors for NIR imaging of neutrotransmitters and pathogenic bacteria. Furthermore, present challenges and opportunities for the development of smart surfaces and sensing approaches.

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18

Chirality-induced electron spin polarization in chiral CuO and CoO_x catalyst surfaces

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Spin-polarized catalytic surfaces can greatly enhance the selectivity of chemical reac-tions, e.g., in a photoinduced water splitting process. The introduction of a chiral catalyst surface can generate this spin polarization by means of the chirality-induced spin selectivity (CISS) effect. [1]
Here, we confirm that spin-polarized (photo)currents can be obtained from chiral cupric oxide (CuO) [2] and cobalt oxide (CoO_x) [3] films, and explore the underlying mechan-ism. Chiral oxide films were electrochemically deposited on polycrystalline gold sub-strates using a method pioneered by Switzer et al. [4] Photoelectrons were excited with deep-UV laser pulses, and their average spin polarization was measured.
For thin CuO films, the spin polarization exceeds $P = -10\%$ with 'L' chirality and, notably, is reversed for oxide films of opposite 'D' chirality. Correlation of the spin polar-ization values with electron energy spectra indicates that the measured polarization values can be rationalized assuming an intrinsic spin polarization in the chiral oxide layer and a CISS-related spin filtering of electrons. On chiral CoO_x layers, the spin polarization was found to depend on the cobalt 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. This sensor will be integrated into a synthetic hydrogel in which cells can live in a 3D environment so that mechanical signals exerted by the cells can be quantified with fluorescence lifetime imaging (FLIM). However, one limitation of the current tension sensor-setup is a small signal-to-noise ratio which aggravates the readout in complex 3D 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 (μs)-range and thereby enhance the dynamic range of the tension sensor. Finally, these components need to be incorporated into the synthetic hydrogel and by gradually increasing the complexity of the hybrid material, responsive and adaptive features can be incorporated.

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H-Bonded Ambipolar Supramolecules for Room Temperature Ferroelectricity

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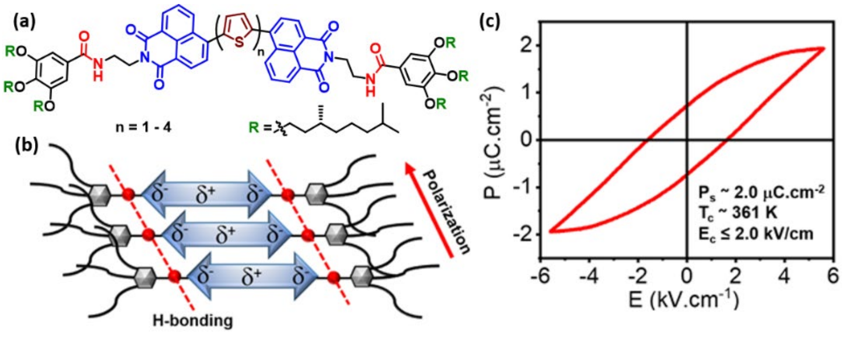
Ferroelectric (FE) materials possess spontaneously generated reversible electric polarization with applications ranging from electronics to electromechanics. Recent advancements in microelectronics or mechano-bio interactive sectors demand for soft FE-materials as they offer better processability and flexible device fabrication. However, most organic FE-systems exhibit low-to-moderate polarization at ambient condition and are not comparable with the state-of-the-art inorganic perovskites or hybrid materials. Considering the requirement of sequence dependent stacking of micro-dipoles and long-term stability, we envisaged that the intrinsic polarizability of self-assembled ambipolar chromophores could be explored for FE-switching. To this quest, we have studied four ambipolar supramolecules (Figure 1a) in which naphthalimide and oligothiophene serve as the acceptor (A) and donor (D) units, respectively. They are equipped with amide functionality for H-bonding driven supramolecular polymerization. In the assembled state, AD_1A and AD_2A exhibit bathochromically shifted absorption bands while AD_3A and AD_4A show H-aggregation with hypsochromic shift. Polarization vs. electric field (P-E) measurements reveal stable rt ferroelectricity, most prominent for the AD_2A system, with a Curie temperature (T_c) of 361 K and saturation polarization (P_s) of 2.0 □C.cm^{-2} at a low coercive field of 2.0 kV.cm^{-1}. Control molecules, lacking either D-A chromophore or amide groups, do not show any ferroelectricity, vindicating the present supramolecular design.

Figure 1. *(a) Generalized structure of the bis-amide functionalized AD_nA molecules; (b) Schematic representation of the H-bonded supramolecular polymerization and (c) a representative P-E loop.*



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Developing tunable triplet emitters towards adaptive electroluminescent materials

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For metal-complex based responsive materials, multiple approaches are viable. We decided to use Pt(II)-complexes with a tridentate CNN luminophore and an exchangeable fourth coordination position. First, we designed the main ligand with the purpose to enable aggregation as a possible readout. Afterwards, we exchanged the remaining chlorido-coligand for a pyridine to test the reaction conditions for an embedding in a pyridine-based polymer in collaboration with the Gröschel group. To get a photoresponsive material, we thought to use azo-based co-ligands, due to their defined photoswitch and guest-host chemistry.

We have developed reactive (ReaxFF) force fields for nonadiabatic simulations of the photoisomerization of azo-compounds within such complex systems. Unlike classical force fields, reactive force fields can handle bond breaking and formation and adapt to changing chemical environments. The force field parameters are fitted to ab initio reference data for both ground and first excited state of azobenzene derivatives, as well as ground state properties of a variety of other small molecules to ensure a wide range of applications and compatibility with existing force fields. Combining the representations of electronic states with a surface hopping model, we simulate azobenzene derivatives in different solvents and on surfaces.

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Programmable control of gene expression using non-natural AdoMet analogs

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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 transcriptionor 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] MATs are self-regulated by product inhibition through AdoMet (or analogs). This can be circumvented when directly coupling methyltransferases (MTases) to the MAT reaction.[2] MTases use AdoMet as cofactor to methylate biomolecules. Usage of promiscuous MTases allows transferring non-natural groups to nucleic acids to regulate their functionalities.[3] In addition to MAT/MTase cascade reactions, riboswitches can influence gene expression as they actuate protein production when sensing AdoMet,[4] creating another important output signal depending on the AdoMet level.

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23

Ultra fast dynamics in thiophene-based conjugated donor-acceptor organic polymers for photovoltaics

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Thiophene-based polymers are promising candidates for solar cell, OLED or transistor (OFET) applications. An internal donor (D) – acceptor (A) system is formed by coupling thiophene polymers with pyrrole chains. The charge transport behavior can be tuned by different alkyl side chains since they influence the electronic structure, HOMO and LUMO level positions, and interchain interactions. A direct assessment of the intramolecular and intermolecular dynamics may guide synthesis routes. With diketopyrrolopyrrole – quaterthiophene (PDPP4T) and thienyl-diketopyrrolopyrrole-thienothiophene (PDPPTTT) we investigated the electronic dynamics of verified high hole-mobility organic semiconductors. For the second polymer, the two thiophene rings were exchanged for thienothiophene in the backbone. In contrast, another polymer pF8T2 with bi-thiophene in the backbone was used, but with fluorene instead of pyrrole as acceptor. These different molecular configurations are intended to provide insights into the change in electron configuration due to both backbone modification and intermolecular packing.

We report results of temporally resolved photoemission studies on thiophene polymers on Si(100) substrates. Occupied electronic levels were analysed via static UPS. Dynamic 2PPE experiments were performed for the energetic position and dynamics of the unoccupied states. Details in the electron dynamics were resolved with the fourth harmonic of a 500 kHz fiber laser as probe pulse and IR and UV radiation from a NOPA as pump pulse.

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SmartMatters4You

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SmartMatters4You is a project on intelligent matter for female students in upper school and first year at the university. Participants take part in numerous hands-on laboratory visits and excursions. In interdisciplinary workshops, organized and conducted by the student laboratory MExLab Physik, they can experience access to the field of intelligent matter.

The natural sciences are still less studied by women than by men – this gender gap is a massive problem that runs through society right up to the management level. For instance, only 16% of all artificial intelligence specialists in Germany are female[1]. Not only is this wasted potential, but it can also amplify the problem when algorithms created by men reproduce stereotypes[2].

This is where the project comes in by drawing attention to the issue of gender equality. More female role models in the STEM fields are needed[3]. 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 an accompanying study, the mechanisms of the career choice decisions of high school students and the role of social barriers such as stereotypes are examined using methods of empirical social research.

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Emissive alcohol low molecular weight gelators

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Supramolecular gels are soft materials based on the non-covalent interaction of small molecules (Low-molecular-weight-gelators, LMWGs).[1] In contrast to their polymer-based, covalent relatives, they are more sensitive to influences from the outside, which opens the wide field of sensing-applications and material sciences, but moreover can be easily functionalized to gain more interesting properties.[2] One of these features is the so-called aggregation-induced emission (AIE), firstly described in 2001 by Ben Zhong Tang, which described the appearance of luminescence upon restriction of intramolecular motion.[3] The combination of these two enables a new kind of functional material with different read-outs for sensing applications.[4]

In the presented work we synthesized a small library of eight possible LMWGs based on estrone, bearing AIE-properties in the gel-state. Upon screening common lab-used solvents, fast gelation could only be observed for alcohols while few gels were obtained only over several weeks in other solvents. Critical gel-concentrations and temperatures were determined as well as their photophysical properties.

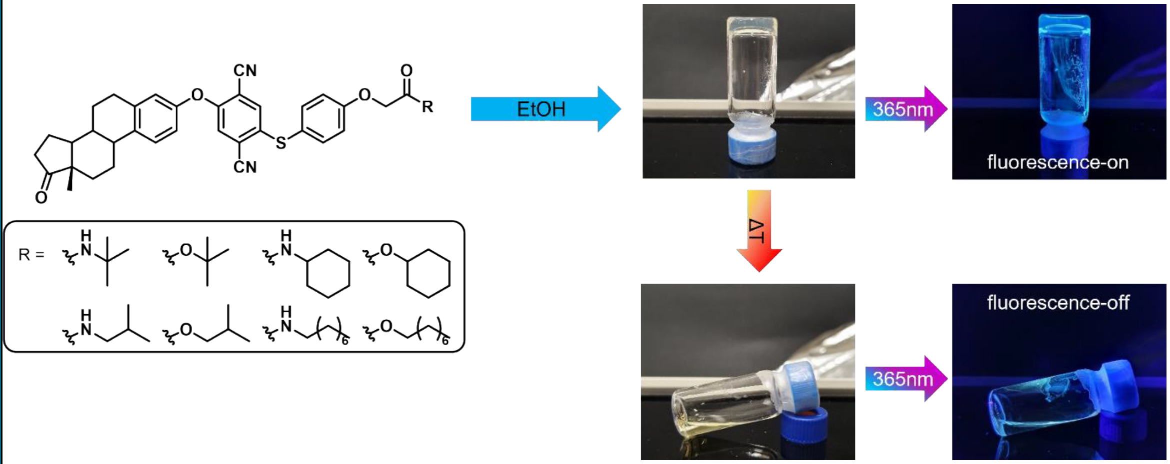

Figure 1. Estrone-based LMWG library (left) forming organo-gels with AIE-properties in EtOH.

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26

Towards intelligent light-propelled nano- and microsystems

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Suspensions of self-propelled particles represent a novel class of matter exhibiting many promising properties useful in fields like microfabrication or biomedicine. The continuous external supply of energy gives rise to several collective phenomena unseen in passive matter such as motility induced phase separation. Here we present a refraction-based approach to particle propulsion using symmetry-broken refractive index profiles. Compared to simple short-range repulsion the particle interaction is significantly more complex as refractive particles can interact indirectly via the light field. The combination of responsiveness to an external light field, complex constituent interaction and inertial memory makes this approach a prime candidate for intelligent matter.

Since analytical theories for these particle systems are still under development, extensive numerical simulations are needed to design particles for a desired collective behavior. Here we present a novel framework for simulating particle dynamics, a general approach to soft interactions between arbitrarily shaped particles and a ray tracing software for estimating forces and torques on refractive particles.

For fabrication of light-driven particles in form of microswimmers femtosecond laser-based manufacturing by two-photon polymerization is exploited. This technique enables the realization of arbitrary three-dimensional particle shapes and tailored refractive index gradients. We demonstrate the directional propulsion of asymmetric microswimmers and the increased forces with the addition of refractive index gradients.

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Breakdown of dipolar blueshift at low-temperatures indicating quantum correlations in exciton ensembles in WSe_2-$MoSe_2$ hetero-bilayer

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Atomistic van der Waals hetero-bilayers are ideal systems to study the (quantum-) phase diagram of excitons including Bose-Einstein condensation due to large exciton binding energies, an interfacial dipole moment and long lifetimes[1,2]. Light emission and electron energy-loss spectroscopy showed first evidence of excitonic many-body states in such two-dimensional materials[3,4]. Pure optical studies have been elusive.
We observe several criticalities in photogenerated exciton ensembles hosted in $MoSe_2$–WSe_2 hetero-bilayers with respect to emission intensity, linewidth, and temporal coherence pointing towards a coherent many-body state[5]. For this state, the estimated occupation is approximately 100%. Most intriguing, the density dependent dipolar blueshift breaks down at millikelvin temperatures over at least 5 orders of magnitude of the excitation fluence indicating transition to a quantum liquid phase[6].

We acknowledge support by DFG and SPP2244.

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28

Photoinduced synthesis of luminescent dibenzothiophenes in polymer matrices

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The heterocyclic dibenzothiophene (DBT) moiety exhibits favourable charge transfer properties and can facilitate intersystem crossing (ISC) via n-π*-transitions, hence a variety of optoelectronic materials like OLED or semiconductors make use of this motif.[1] The most common syntheses of functionalized DBT derivatives rely on transition metal catalysis and provide di- or trisubstituted DBT.[2]

In the work presented here, a photochemical cyclization reaction of aromatic thioethers that leads to highly substituted DBT is described. Using analytical HPLC, the reactivity of different (thio-)ethers was investigated to shed light on the underlying mechanism. By performing the reactions on a preparative scale, the photophysical properties of the products could be examined.

We found that the position of electron donating and accepting groups plays a major role for the reactivity, indicating an internal charge transfer mechanism. The cyclization influences the fluorescence behaviour of the luminophores both in the solid state and in solution. Furthermore, the reaction can be induced in polymer films, which allows for the inscription of phosphorescent motifs.

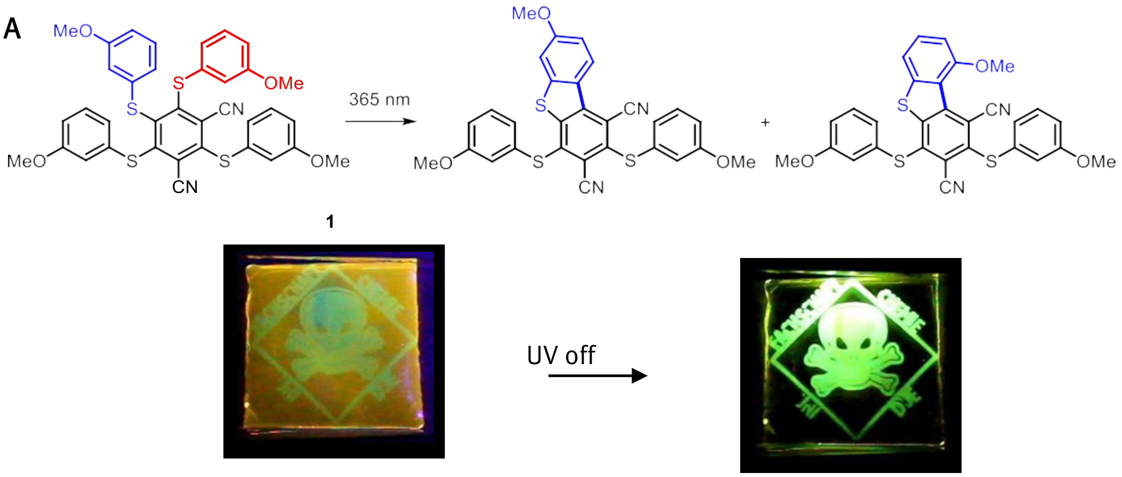

Figure 1. **A** Exemplary reaction scheme for the photoinduced cyclization of an aromatic thioether. **B** Phosphorescence of a polymer film containing **1**. The motif was inscribed via irradiation using a template.

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29

Dual-functional memory behavior in EGaIn-PEDOTPSS-Au devices

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Alternative organic electronic memory devices, functioning as neuromorphic and/or one diode-one resistor (1D-1R) systems can help overcome the limitations faced by conventional semiconductor technology.[1] Thin films of PEDOT:PSS have been well explored in thermoelectric, LEDs, solar cells, and recently in neuromorphic devices.[2] Here, we demonstrate the working of PEDOT:PSS devices (Fig. 1a) functioning as excellent 1D-1R diodes with abnormal electrical hysteresis, wherein the corresponding rectification and conductance ratio of the ON and the OFF states were found to be as high as ~10^7 and ~10^5, respectively (Fig. 1b). Furthermore, we investigated the durability and memory retention of these devices by performing large numbers of WRER cycles. Finally, we aim to fabricate crossbar devices to kill sneak-path currents and show enhanced device functioning.

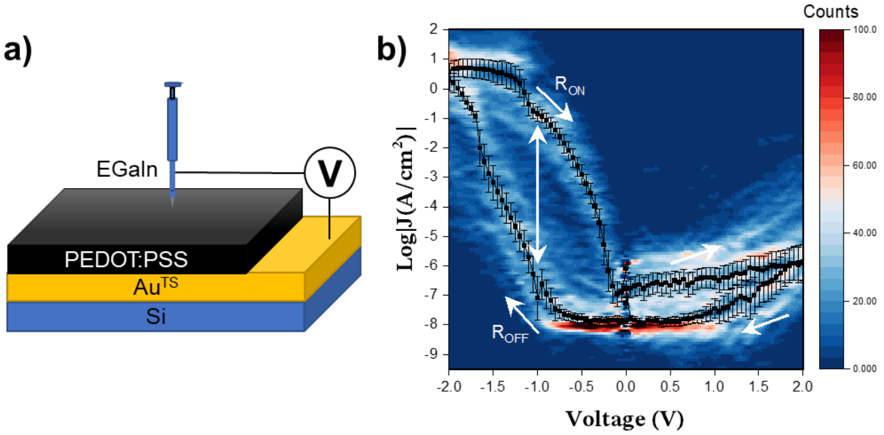

Figure 1. a) Schematic of a device comprising of spincoated film of PEDOT:PSS on Au^{TS} and with EGaIn (eutectic Gallium-Indium alloy) as top electrode, **b)** Semilog plot of current density vs. voltage (Log|*J*|-*V*) showing high rectification and hysteresis. The black squares represent the mean of Log|*J*|, with the heatmap of raw data in background.

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Light-controlled anion binding 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]

Here we first point out a general caveat in anion binding studies, occuring at poor salt dissociation. By determining electrophoretic mobilities of the involved species, a model which takes the salt dissociation equilibrium into account yields corrected binding constants. We furthermore modify the host structure by including an azobenzene unit to effectively switch between its cis and trans conformation by light irradiation. 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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Exciton species in highly doped WS_2 monolayers

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Semiconducting two-dimensional transition metal dichalcogenides such as WS_2 excel due to their exciton dominated light-matter interaction even at room temperature (RT) that is highly tunable by external stimuli such as doping, light excitation, dielectric environment, or strain [1]. In this work, an optimized field effect structure utilizing a polymer electrolyte top gate electrode is employed to study the evolution of the optical response in monolayer WS_2 at RT in dependence of doping by means of photoluminescence, spectroscopic imaging ellipsometry and Raman measurements. The huge geometrical gate capacitance enables capacitance spectroscopy of the conduction band as well as valence band edge yielding a gap energy of ~2.6eV in agreement with the determination from the exciton Rydberg series. The gate allows the injection of large electron and hole densities exceeding $10^{14} cm^{-2}$, sufficient to enable the exciton Mott transition. The obtained doping dependent emission and absorption spectra also facilitate the identification of phonon activated, neutral and charged exciton species as well as dressed excitons in a fermi sea.

We acknowledge financial support via DFG WU 637/7-1 and SPP2244.

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Mixed-mode in-memory computing using adaptive 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 is using programmable phase-change devices at the cross points to represent the matrix elements. Light travelling through the waveguide couples evanescently to the PCM. 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, cyclability 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 PIN heater. This way, we hope to achieve excellent control over the transmissive state and a large switching contrast. As a next step, these mixed-mode devices are then implemented into waveguide arrays. On this poster, we present the first steps in the development of the mentioned electro-optical phase-change devices.

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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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Photolithography with green to far-red light for protein micro patterns

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Protein micro patterns are important for screening arrays and controlling cell material interactions. A few methods allow patterning functional proteins with noninvasive visible light yet none are work with red or far-red light and allow co-patterning multiple proteins. Herein, we report multi-color photolithography for protein patterning with green, red and far-red light. For this purpose, we used the green light cleavable protein CarH, which is a tetramer in the dark in the presence of its cofactor 5'-deoxyadenosylcobalamin (AdoB12) and dissociates into its monomers under green light illumination. By adding the dyes cyanine 5.5 and cyanine 7.5-encoded to AdoB12, the CarH became responsive to red and far-red light, respectively. These new versions of CarH were incorporated into a layer-by-layer (LbL) multi-protein film as photosensitive layers using interaction between His-tags on the proteins and Ni^{2+}-NTA groups. The specific removal of upper layers was possible through the illumination with green light, red light and far-red light in any desired combination. This multi-color lithography provides a mild and flexible way to micro-pattern poly-His-tagged proteins with high spatiotemporal control. Also provides a reliable strategy for protein patterning with potential applications in biotechnology.

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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 Mn 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 photo-isomers 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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