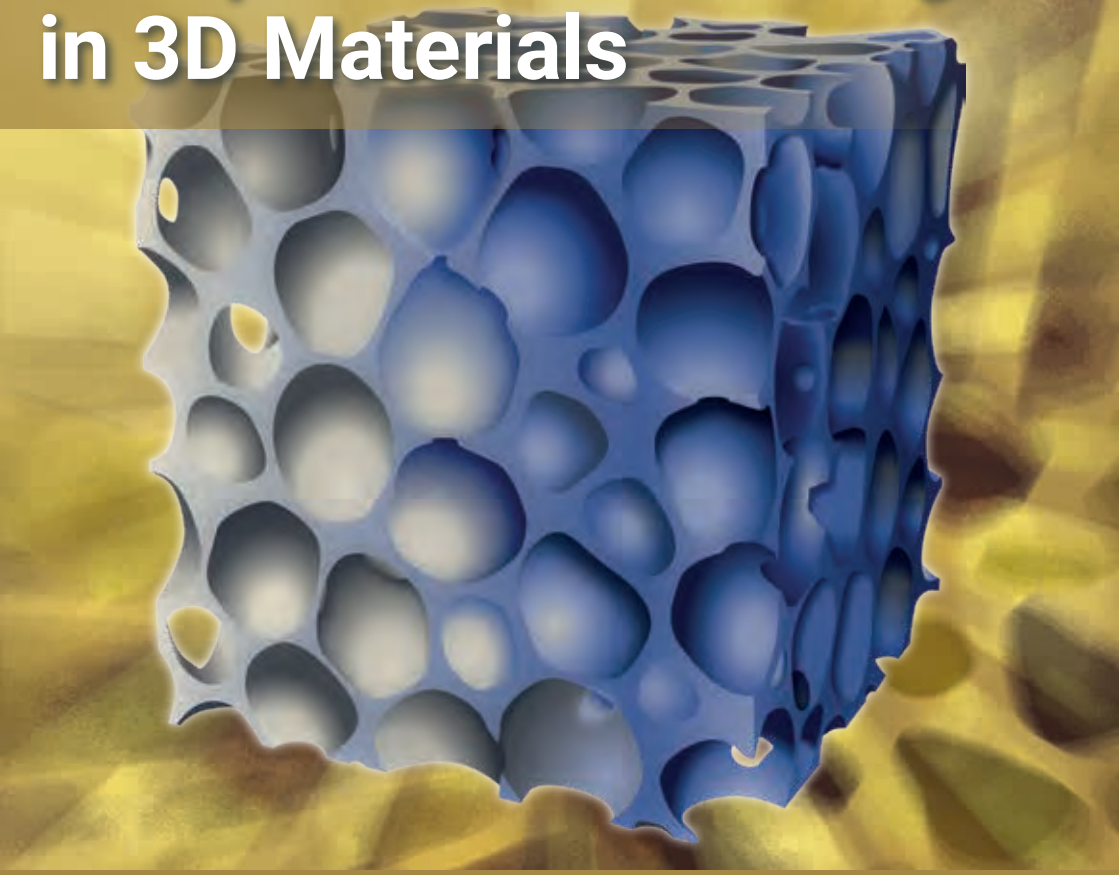
Frontiers for Theory, Computation and Design in 3D Materials



Abstract Booklet

March 23 – 25, 2026

Schöntal Monastery, Germany

Content

Welcome

Dear Colleagues and Friends,

We are delighted to welcome you to

The Future 3D Additive Manufacturing – The 3DMM2O Conference 2026: Frontiers for Theory, Computation and Design in 3D Materials.

The annual conference on topics surrounding 3D Additive Manufacturing is organized by the Cluster of Excellence "3D Matter Made to Order" (3DMM2O). 3DMM2O is a joint Research Cluster of Karlsruhe Institute of Technology (KIT) and Heidelberg University (Uni HD).

The conference shall be a platform for new approaches in the field of 3D Additive Manufacturing. It aims to connect theory, computation, and design to advance next-generation 3D materials and push the boundaries of additive manufacturing beyond conventional approaches.

Lectures by national and international speakers, as well as poster sessions, will give you insight into various aspects of 3D Additive Manufacturing. Social networking events and coffee breaks will foster inspiring and fruitful scientific discussions and exchange.

Enjoy the conference amidst the stunning and historic surroundings of Schöntal Monastery!

Carsten Rockstuhl
Karlsruhe Institute of Technology (KIT)

Ulrich Schwarz
Heidelberg University (Uni HD)

Wolfgang Wenzel
Karlsruhe Institute of Technology (KIT)

Program

TIME	ROOM		
4:00 PM	Entrance Schöntal Monastery	Check-In	SUNDAY MARCH 22
6:00 PM–8:00 PM	Dining Hall (ground floor)	**Dinner at Individual Time**	
8:00 PM	Abt Knittel Keller (basement)	Informal Get-Together	

			MONDAY MARCH 23
	Dining Hall (ground floor)	**Breakfast**	
9:00 AM–9:05 AM	Banquet Hall (2nd floor)	Opening & Welcome	
9:05 AM–9:45 AM		Designing 3D Manufacturable Metamaterials	**Martin Wegener**
9:45 AM–10:25 AM		High-Speed X-Ray Tomography for 4D Imaging	**Vikram Deshpande**
10:25 AM–10:40 AM	219	**Coffee Break**	
10:40 AM–10:55 AM	Banquet Hall (2nd floor)	**Contributed Talk:** Dynamic Control of Rigidity Via Geometric Frustration in Stimuli-Responsive Mechanical Metamaterials	**Santiago Gomez Melo**
10:55 AM–11:10 AM		**Contributed Talk:** Geometry Screening of a 3D-Printed Biocatalytic Reactor	**Bruno Vuillod**
11:10 AM–11:50 AM		Combinatorial Metamaterials: From Spin Ice to Novel Mechanical Functionalities	**Yair Shokef**
11:50 AM–12:00 PM	Entrance Schöntal Monastery	Group Picture	
12:00 PM–1:30 PM	Dining Hall (ground floor)	**Lunch**	
1:30 PM–2:10 PM	Banquet Hall (2nd floor)	Topological Defect Engineering Enables Size and Shape Control in Self-Assembly	**Martin Lenz**
2:10 PM–3:00 PM		Wavelength-Resolved Photochemical Reactivity Dictated by Microenvironments	**Christopher Barner-Kowollik**
3:00 PM–3:20 PM	219	**Coffee Break**	
3:20 PM–4:00 PM	Banquet Hall (2nd floor)	Cluster-Based Materials *in Vitro* and *in Silico*	**Stefanie Dehnen**
4:00 PM–4:40 PM		Programming Biological Shapes: Morphogenesis in an Active Solid	**Carl Modes**
4:40 PM–5:00 PM	219	**Coffee Break**	
5:00 PM–5:10 PM	Banquet Hall (2nd floor)	Flashtalks	
5:10 PM–6:00 PM	203 & 204	Poster Session I	
6:30 PM	Dining Hall (ground floor)	**Dinner**	
8:00 PM–8:40 PM	Banquet Hall (2nd floor)	Why Inverse Design Should be Unphysical	**Steven G. Johnson**

		TUESDAY MARCH 24	
	Dining Hall (ground floor)	**Breakfast**	
9:00 AM–9:40 AM	Banquet Hall (2nd floor)	A Hybrid Automated and Autonomous Workflow to Discover High Performance Semiconductors for Photovoltaics	**Christoph Brabec**
9:40 AM–10:20 AM		Digital Catalysis: When the Algorithms Take Over	**Christoph Scheurer**
10:20 AM–10:35 AM	219	**Coffee Break**	
10:35 AM–11:15 AM	Banquet Hall (2nd floor)	Unveiling the Dynamics in Functional Materials at the Atomistic Level	**Saeed Amirjalayer**
11:15 AM–11:30 AM		**Contributed Talk:** Multiscale Modelling of the Linear and Nonlinear Optical Response of Molecular Materials and Devices Thereof	**Marjan Krstić**
11:30 AM–11:45 AM		**Contributed Talk:** Design Optimization of Printed Thermoelectric Generators for Energy Harvesting and Waste Heat Recovery	**Muhammad Irfan Khan**
11:45 AM–12:00 PM		**Contributed Talk:** Structural Flexibility Explains Solvent-Induced Spectral Shift in Styrylpyrene	**Samira Gholami**
12:00 PM–1:30 PM	Dining Hall (ground floor)	**Lunch**	
1:45 PM–2:00 PM	Entrance Schöntal Monastery	Meet for Social Program	
2:00 PM–6:00 PM		Social Program	
7:00 PM	Banquet Hall (2nd floor)	**Conference Dinner**	

WEDNESDAY MARCH 25

	Dining Hall (ground floor)	**Breakfast**	
9:00 AM–9:40 AM	Banquet Hall (2nd floor)	Molecular-Plasmonic Hybrid Systems – a Theoretical Description Accessing the Chemical and Electromagnetic Contributions	**Stefanie Gräfe**
9:40 AM–10:20 AM		Advances in Topology Optimization for Metaphotonics	**Antonio Calà Lesina**
10:20 AM–10:35 AM	219	**Coffee Break**	
10:35 AM–11:15 AM	Banquet Hall (2nd floor)	Combining Data-Driven and Physics-Based Approaches to Predict, Understand, and Control Active Matter Dynamics	**Mike Hagan**
11:15 AM–11:55 AM		Towards an Artificial Muse for New Ideas in Physics	**Mario Krenn**
12:00 PM–1:30 PM	Dining Hall (ground floor)	**Lunch**	
1:30 PM–1:45 PM	Banquet Hall (2nd floor)	**Contributed Talk:** Deep Learning-Based Inverse Design of Holographically Produced 3D Photonic Metamaterials with Tailored Photon Density of States	**Zesen Zhou**
1:45 PM–2:25 PM		Supramolecular Design Principles for Material–Cell Communication	**Tanja Weil**
2:25 PM–3:05 PM		Computational Modelling of Animal Development	**Erika Tsingos**
3:05 PM–3:20 PM	219	**Coffee Break**	
3:20 PM–3:30 PM	Banquet Hall (2nd floor)	Flashtalks	
3:30 PM–4:20 PM	203 & 204	Poster Session II	
4:20 PM–4:30 PM	219	**Coffee Break**	
4:30 PM–5:10 PM	Banquet Hall (2nd floor)	Machine Learning for Molecules and Materials – From Property Prediction and Design to Understanding	**Pascal Friederich**
5:10 PM		Closing Words	
6:00 PM	Dining Hall (ground floor)	**Dinner**	

THURSDAY MARCH 26

Until 9:00 AM		Check-Out, **Breakfast,** Departure	

Speakers' Abstracts

In Alphabetical Order

Tuesday, March 24
10:35 AM–11:15 AM

Saeed Amirjalayer

Heidelberg University, Germany

UNVEILING THE DYNAMICS IN FUNCTIONAL MATERIALS AT THE ATOMISTIC LEVEL

Responsive and functional materials exhibit complex, often nonlinear behaviour when subjected to external stimuli such as light, mechanical force, temperature and chemical environments. Understanding the underlying dynamic phenomena that govern their responses is crucial for engineering materials for applications such as actuation, information storage, catalysis and energy conversion.

In this presentation, I will provide a selective overview of our work on developing and applying theoretical methods in atomistic investigations of functionalized surfaces, molecular crystals and porous materials. I will discuss the impact of intermolecular interactions and confinement on individual, coupled and collective dynamics. Using representative examples, I will highlight how we can obtain a comprehensive insight into these systems by combining our atomistic simulations with advanced experimental techniques.

Christopher Barner-Kowollik

Karlsruhe Institute of Technology (KIT), Germany

WAVELENGTH-RESOLVED PHOTOCHEMICAL REACTIVITY DICTATED BY MICROENVIRONMENTS

When selecting a light source for a photochemical process – including for photopolymerizations – we often consider the likelihood of a photon to be absorbed by a chromophore at a given wavelength as an accurate predictor of how well a photochemical process will proceed when irradiated with different colors of light.

Over the last decade this paradigm has been repeatedly challenged for several photochemical reactions, as a distinct mismatch between the absorption spectrum and the wavelength resolved photochemical reactivity has been observed. Herein, we unravel potential underlying mechanisms behind the mismatched reactivity and absorbance in photocycloadditions. Initially, we probe the impact that an equilibrium established between reversible photochemical processes has on the mismatch for a pyrene-chalcone molecule.

Subsequently, we establish a critical link between photophysics and photochemistry with a theory based on the selective excitation of specific microenvironments leading to molecular transitions that allow for favourable wavelength-dependent reactivity. Time-resolved and steady-state fluorescence spectroscopy measurements confirm the presence of this selectivity, with both displaying significant red-edge effects that are observed in fluorescence spectroscopy literature, further supporting our theory.

By synthetically tethering chromophores together, we further evidence the importance of microenvironments and their wavelength-dependent excited-state lifetimes, presenting the missing link that explains the mismatch for many photochemical systems.

The implications of the theory presented herein stretch from additive manufacturing to photo-dynamic therapy, meaning that we can potentially leverage photochemical mismatches by changing the properties of the environment surrounding the chromophore.

Carrol, J. A.; Pashley-Johnson, F.; Klein, M.; Stephan, T.; Pandey, A. K.; Walter, M.; Unterreiner, A. N.; Barner-Kowollik, C. J. Am. Chem. Soc. 2025, 147, 26643-26651.
Pashley-Johnson, F.; Wu, X.; Carroll, J. A.; Walden, S. L.; Frisch, H.; Unterreiner, A. N.; Du Prez, F. E.; Wagenknecht, H. A.; De Alaniz, J. R.; Feringa, B. L.; Heckel, A.; Barner-Kowollik, C. Angew. Chem. Int. Ed. 2025, 64, e202502651.

Speakers'

Tuesday, March 24
9:00 AM–9:40 AM

Christoph J. Brabec

Friedrich-Alexander-University Erlangen-Nürnberg, Germany

A HYBRID AUTOMATED AND AUTONOMOUS WORKFLOW TO DISCOVER HIGH PERFORMANCE SEMICONDUCTORS FOR PHOTOVOLTAICS

The inverse design of tailored organic molecules for specific optoelectronic devices of high complexity holds an enormous potential but has not yet been realized. Current models rely on large data sets that generally do not exist for specialized research fields. We demonstrate a closed-loop workflow that combines high-throughput synthesis of organic semiconductors to create large data sets and Bayesian optimization to discover new holetransporting materials with tailored properties for solar cell applications. The predictive models were based on molecular descriptors that allowed us to link the structure of these materials to their performance. A series of high-performance molecules were identified from minimal suggestions and achieved up to 26.2% (certified 25.9%) power conversion efficiency in perovskite solar cells. Similar models based on the Bayesian theorem are now available to resolve high-dimensional optimization challenges, including the full processing of solar cells and even tandem cells. The success of these models is demonstrated at the hand of high reproducibility and performance, as in the case of perovskite single junction cells with efficiencies beyond 27 %.

This presentation will give an overview on autonomous operating self-driven labs for photovoltaics, showing how synthesis, film formation, microstructure formation, device processing and lifetime testing can integrated into one platform.

Abstracts

Stefanie Dehnen

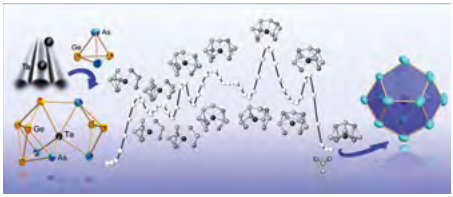
Karlsruhe Institute of Technology (KIT), Germany

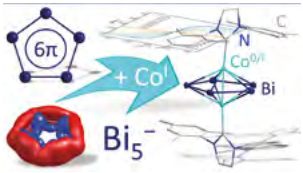
CLUSTER-BASED MATERIALS *IN VITRO* AND *IN SILICO*

The diversity of cluster compositions and architectures largely affects the chemical and physical properties of materials based on them, which has stimulated research in this field worldwide—both regarding the synthesis of corresponding compounds and the theoretical work associated with those efforts.[1] In particular, clusters that combine main group elements of the p-block with atoms from the d- or f-block metals have been a source of inspiration over the years and keep enjoying a lot of attention.[2–4]

In addition to fundamental aspects, such as the interactions between heavier elements and insights into the still only fragmentarily explored formation of multimetallic clusters (see figure, left),[5–7] such species are intensely studied in regards of cluster-based bond activation,[8] or as precursors for new intermetallic nanoarchitectures.[9] The inclusion of open-shell d- or f-block metal atoms in such clusters can lead to substantial ring currents and aromatic behavior as a response to magnetic fields. Such features were recently discussed for $[U@Bi_{12}]^{3-}$,[10] $[Th@Bi_{12}]^{4-}$,[11] $[\{CpRu\}_3Bi_6]^-$,[12] and the Bi_5^- anion trapped for the first time in $[\{IMesCo\}_2Bi_5]$ (see figure, right).[13] For all these investigations, computational work constitutes an indispensable tool.

The processes often proceed on timescales too short to be captured experimentally, occur under conditions that are challenging to access (for example, within a high-temperature furnace), or involve compounds that lack a suitable spectroscopic or chemical handle to monitor their transformation or properties in solution. Consequently, in this domain of inorganic chemistry and materials research, in vitro and in silico approaches are inherently intertwined in a fundamentally synergistic manner.





[1] Zhang, J.; Bu, X.; Feng, P.; Wu, T. Acc. Chem. Res. 2020, 53, 2261.
[2] Wilson, R. J.; Lichtenberger, N.; Weinert, B.; Dehnen, S. Chem. Rev. 2019, 119, 8506.
[3] McGrady, J. E.; Weigend, F.; Dehnen, S. Chem. Soc. Rev. 2022, 51, 628.
[4] Pan, F.; Peerless, B.; Dehnen, S. Acc. Chem. Res. 2023, 56, 1018.
[5] Mitzinger, S.; Broeckaert, L.; Massa, W.; Weigend, F.; Dehnen, S. Nat. Commun. 2016, 7, 10480.
[6] Pan, F.; Wei, S.; Guggolz, L.; Eulenstein, A. R.; Tambornino, F.; Dehnen, S. J. Am. Chem. Soc. 2021, 143, 7176.
[7] Townrow, O. P. E.; Weller, A. S.; Goicoechea, J. M. Angew. Chem. Int. Ed. 2024, 63, e202316120.
[8] Townrow, O. P. E.; Chung, C.; Macgregor, S. A.; Weller, A. S.; Goicoechea, J. M. J. Am. Chem. Soc. 2020, 142, 18330.
[9] Bentlohner, M. M.; Waibel, M.; Zeller, P.; Sarkar, K.; Müller-Buschbaum, P.; Fattakhova-Rohlfing, D.; Fässler, T. F. Angew. Chem. Int. Ed. 2016, 55, 2441.
[10] Lichtenberger, N.; Wilson, R. J.; Eulenstein, A. R.; Massa, W.; Clérac, R.; Weigend, F.; Dehnen, S. J. Am. Chem. Soc. 2016, 138, 9033.
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[12] Peerless, B.; Schmidt, A.; Franzke, Y. J.; Dehnen, S. Nat. Chem. 2023, 15, 347.
[13] Rienmüller, J., Peerless, B., Paul, S.; Bruder F.; Wernsdorfer, W.; Weigend. F.; Dehnen S. Nat. Chem. 2025, 17, 547.

Speakers'

Monday, March 23
9:45 AM–10:25 AM

Vikram Deshpande

University of Cambridge, United Kingdom

HIGH-SPEED X-RAY TOMOGRAPHY FOR 4D IMAGING

Capturing high-rate spatiotemporal deformation of materials in three dimensions (3D) remains a significant challenge with current X-ray imaging techniques.

We present a methodology that combines advances in neural rendering techniques with volume correlation methods to accurately reconstruct complex, high-rate 3D spatiotemporal structural evolutions. The fidelity and versatility of the method, which requires no pre-training, are demonstrated for a diverse set of intricate 3D-printed micro-architected solids.

Using laboratory-based X-ray tomography, we capture the 3D growth of a dynamic crush band on a timescale of less than 100 milliseconds. By broadening this idea to a stereo X-ray concept, we eliminate the need to rotate the image object, thereby extending the technique to significantly faster timescales.

Our neural rendering framework opens new possibilities for studying numerous poorly understood dynamic processes, such as the runaway failure of batteries and the temporal evolution of 3D shock microstructures under impact loading, all using laboratory X-ray systems.

Pascal Friederich

Karlsruhe Institute of Technology (KIT), Germany

MACHINE LEARNING FOR MOLECULES AND MATERIALS - FROM PROPERTY PREDICTION AND DESIGN TO UNDERSTANDING

Machine learning can accelerate the screening, design, and discovery of new molecules and materials in multiple ways, e.g. by virtually predicting properties of molecules and materials, by extracting hidden relations from large amounts of simulated or experimental data, or even by interfacing machine learning algorithms for autonomous decision-making directly with automated high-throughput experiments.

In this talk, I will focus on our research activities on materials property prediction [1,2] and inverse design of materials [3], materials foundation models [4], as well as self-explaining graph neural networks [5,6] to foster scientific understanding in chemistry and materials science.

[1] Ruff et al., Digital Discovery 3, 594-601, 2024.
[2] Reiser et al., Communications Materials 3, 93, 2022.
[3] Ruple et al., arXiv:2502.03146, under review.
[4] Mirza et al., ICLR AI4MAT Workshop, 2025.
[5] Teufel et al., Explainable Artificial Intelligence 2023 1902, 338-360
[6] Sturm et al., Angewandte Chemie 2025.

Speakers'

Wednesday, March 25
9:00 AM–9:40 AM

Stefanie Gräfe

Friedrich Schiller University Jena, Germany

MOLECULAR-PLASMONIC HYBRID SYSTEMS – A THEORETICAL DESCRIPTION ACCESSING THE CHEMICAL AND ELECTROMAGNETIC CONTRIBUTIONS

The excitation of collective electron dynamics inside the metallic nanoparticles induced by external light fields leads to strongly re-shaped electromagnetic nearfields with a complex spatial and temporal profile. The interaction of these modified and enhanced nearfields with systems located in close vicinity to the metallic nanoparticle is the origin of many astonishing physical and chemical phenomena, such as the formation of new quasiparticles, new mechanisms for chemical reactions or the ultra-high spatial resolution and selectivity in molecular detection.

For the theoretical description of such plasmonic hybrid systems in external light fields, it is necessary to describe both the electromagnetic interaction and the more chemical effects equally.

In this talk, I will introduce our recent results on the theoretical description of these systems, with particular emphasis on spectroscopic applications, e.g., in the context of tip-enhanced Raman scattering spectroscopy and/or plasmon-induced catalysis.

Our calculations show pronounced changes of the Raman spectrum under non-resonant and resonant conditions and support the possibility of sub-nanometer spatial resolution.

Mike Hagan

Brandeis University, USA

COMBINING DATA-DRIVEN AND PHYSICS-BASED APPROACHES TO PREDICT, UNDERSTAND, AND CONTROL ACTIVE MATTER DYNAMICS

Active matter is composed of particles that generate forces or motion, which leads to spectacular emergent dynamics. In principle, active matter could form the basis for a new class of materials with lifelike properties of biological organisms. Yet, active materials exhibit diverse dynamical states, most of which have chaotic dynamics that do not produce work or other useful functions. Thus, a robust control strategy is needed to drive active materials into an emergent state that corresponds to a desirable function. However, designing control protocols requires accurate dynamical models, which are not available for most active matter systems. Developing quantitative models using traditional statistical physics approaches is challenging because active materials lack the scale separation characteristic of equilibrium systems.

In this presentation, I will discuss efforts to combine machine learning, other data-driven techniques, and physics-based models with control theory to address this challenge in the context of a widely-used active material, microtubule-based active nematics. Recent advances in optogenetic motors have enabled constructing the light-activated active nematics, in which the activity can be spatiotemporally controlled by shining light on the sample. The challenge is to determine the spatiotemporal light sequence required to drive the system into a desired behavior. I will describe two complementary approaches to computationally determine an optimal light sequence. In the first, we have adapted a method to discover optimal physics-based continuum models directly from spatiotemporal data, using sparse regression. We have identified several approaches to mitigate measurement errors in the data.

We find that the method can reveal the relative contributions of different physical mechanisms, and quantitatively estimates key experimental parameters. Then, we have developed a framework to combine the optimal physics-based model with optimal control theory to solve for the spatiotemporal activity profile that drives the system into a desired state. We demonstrate that active materials can be driven into arbitrary behaviors, including those which do not correspond to dynamical attractors and thus cannot be accessed without control. Since no model is perfectly accurate for a specific system, in the second approach we develop a deep reinforcement learning (DRL) based controller to enable model-free control of active materials. The controller discovers and implements spatiotemporal sequences of activity to drive a 2D active nematic system toward a prescribed dynamical steady-state.

This framework does not require a detailed physics model, making it ideal for complex active materials that lack quantitative theoretical descriptions. Furthermore, the approach is extremely robust to noise and experimental measurement error. We compare the performance of the physics-based and DRL-based controllers for active nematics.

This work was supported by DE-SC0022291. Preliminary work was supported by NSF DMR-1855914 and DMR-2011846. Computing resources were provided by XSEDE TG-MCB090163 and the Brandeis HPCC (DMR-MRSEC 2011846 and OAC-1920147).

Speakers'

Monday, March 23
8:00 PM–8:40 PM

Steven G. Johnson

Massachusetts Institute of Technology (MIT), USA

WHY INVERSE DESIGN SHOULD BE UNPHYSICAL

Inverse design is the technique of using large-scale optimization (over thousands or even millions of parameters) to allow the computer to "discover" the best arrangement of materials for a given application, often leading to non-intuitive freeform geometries.

The most straightforward way to perform inverse design is to apply optimization to the result of an accurate physical model that directly simulates the desired effect: a "numerical experiment" mirroring (one hopes) the real-world performance.

However, we argue that this is often too restrictive: sometimes, vastly better performance is attainable by allowing the computer to exploit "unphysical" models—inaccurate simulations, unphysical materials, and regimes inaccessible to realistic experiments—as long the eventual result (after optimization convergence) returns to the physical realm.

We illustrate these ideas with several examples from photonics topology optimization, including incoherent emission, laser optimization, and the design of optical filters.

Abstracts

Mario Krenn

University of Tübingen, Germany

TOWARDS AN ARTIFICIAL MUSE FOR NEW IDEAS IN PHYSICS

Artificial intelligence (AI) is a potentially disruptive tool for physics and science in general. One crucial question is how this technology can contribute at a conceptual level to help acquire new scientific understanding or inspire new surprising ideas.

I will talk about how AI can be used as an artificial muse in physics [1], which can design new physics experiments [2,3] or suggest surprising and unconventional ideas and techniques for human scientist [4].

In the end, I will talk about AI-Mandel [5], a closed-loop discovery system that automatically generates new ideas in quantum physics and can execute and verify them with intelligent domain tools, with ideas being at the level of publishable works in quantum physics.

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[2] Ruiz-Gonzalez, Arlt, et al., Digital Discovery of 100 diverse Quantum Experiments with PyTheus, Quantum 7, 1204 (2023).
[3] Krenn, Drori, Adhikari, Digital Discovery of Interferometric Gravitational Wave Detectors, PRX 15, 021012 (2025)
[4] Gu, Krenn, Interesting Scientific Idea Generation Using Knowledge Graphs and LLMs: Evaluations with 100 Research Group Leaders. arXiv:2405.17044 (2024)
[5] Arlt, Gu, Krenn, Towards autonomous quantum physics research using LLM agents with access to intelligent tools. arXiv:2511.11752 (2025).

Speakers'

Monday, March 23
1:30 PM–2:10 PM

Martin Lenz

University of Paris-Saclay (LPTMS), France

TOPOLOGICAL DEFECT ENGINEERING ENABLES SIZE AND SHAPE CONTROL IN SELF-ASSEMBLY

The self-assembly of complex structures from engineered subunits is a major goal of nanotechnology, but controlling their size becomes increasingly difficult in larger assemblies. Existing strategies present significant challenges, among which the use of multiple subunit types or the precise control of their shape and mechanics.

Here we introduce an alternative approach based on identical subunits whose interactions promote crystals, but also favor crystalline defects. We theoretically show that topological restrictions on the scope of these defects in large assemblies imply that the assembly size is controlled by the magnitude of the defect-inducing interaction. Using DNA origami, we experimentally demonstrate both size and shape control in two-dimensional disk- and fiber-like assemblies.

Our basic concept of defect engineering could be generalized well beyond these simple examples, and thus provide a broadly applicable scheme to control self-assembly.

Abstracts

Antonio Calà Lesina

Leibniz University Hannover, Germany

ADVANCES IN TOPOLOGY OPTIMIZATION FOR METAPHOTONICS

Inverse design methods based on topology optimization can uncover nanophotonic structures in 3D with free-form shapes beyond human intuition, and optical functionalities not obtainable with conventional design methods. This talk highlights the recent achievements of my team on large-scale topology optimization for metaphotonics and integrated optics.

Some of the topics include the inverse design of nanostructures made of arbitrary dispersive optical materials, the broadband optimization of absorption in metallic and dielectric nanostructures, anapole effects in plasmonic meta-atoms for transparent metasurfaces and metamaterials, and nanoantennas with desired multipolar response for scattering engineering.

Speakers'

Monday, March 23
4:00 PM–4:40 PM

Carl Modes

Max Planck Institute of Molecular Cell Biology and Genetics (MPI-CBG), Dresden, Germany

PROGRAMMING BIOLOGICAL SHAPES: MORPHOGENESIS IN AN ACTIVE SOLID

Understanding how epithelial sheets of cells robustly and reliably adopt complex shapes during animal development remains a key open problem of developmental biology and tissue mechanics. Classically, cortical contractility of the apical surface of these cells generating local bending moments in an effectively fluid tissue has been the go-to theoretical picture for such problems. However, many morphogenetic events are not well explained under this framework.

We hypothesize that collective, in-plane active cell behaviours could instead generate effective spontaneous strains in a solid tissue and in so doing drive stable shape outcomes. We explore these ideas and their consequences in a series of lower dimensional and/or simplified arenas, from a quasi-1D spontaneous strain buckling instability model of the Drosophila cephalic furrow, to how actively driven neighbour rearrangements in vertex models can give rise both to entropic forces in the tissue and locally establish coarse-grained spontaneous strains at steady state. We then turn to a full-blown 3D problem where, together with experimental collaborators, we show that active, in-plane cellular behaviours create the spontaneous strains that ultimately shape the Drosophila wing disc pouch during the dramatic morphogenetic event known as eversion.

Taken together, these findings establish active, in-plane, solid shape programming as a potentially general mechanism for animal tissue morphogenesis.

Abstracts

Christoph Scheurer

Fritz Haber Institute of the Max Planck Society, Germany

WHEN THE ALGORITHMS TAKE OVER: AI FOR EXPERIMENT PLANNING AND CONTROL

More performant and durable materials are urgently needed to further drive the transition to a sustainable energy system. Unfortunately, accelerated materials discovery is in this field presently still more claim than practical reality. Computational screening approaches hinge on efficient descriptors that only reflect nominal materials properties of the crystalline bulk, simple bulk-truncated surfaces or idealized lattice-matching interfaces. They can thus not account for the substantial, complex and continuous structural, compositional and morphological transitions at the working surfaces or interfaces of functional materials in catalysts, electrolyzers or batteries. Accelerated experimental discovery in turn still suffers from severe throughput limitations, as easily automatable human steps are rarely limiting the overall workflows.

In my talk I will illustrate how the convergence of AI-based experiment planning and control with automation and robotization is currently starting to change this picture. Examples will not only cover straightforward loop-style self-driving labs for direct exploration of design spaces, but also approaches geared toward mechanistic understanding like automated reaction mechanism generation or autonomous electron microscopy.

Methodological frontiers concern significant or varying noise levels (e.g. in case of multi-fidelity measurements), the design of larger numbers of data points (to meet batch-type operation in increasingly parallelized workflows), or agility to either autonomously adapt the shape and dimensions of the search spaces across loops or react to corresponding changes imposed by human scientists.

Speakers'

Monday, March 23
11:10 AM–11:50 AM

Yair Shokef

Tel Aviv University, Israel

COMBINATORIAL METAMATERIALS: FROM SPIN ICE TO NOVEL MECHANICAL FUNCTIONALITIES

Extraordinary responses of mechanical metamaterials often stem from incompatibility of their elementary building blocks. Relying on analogies to magnetic interactions, we describe the deformation fields in complex mechanical metamaterials by discrete spin states.

We show how spin frustration relates to mechanical incompatibility, and we use this to design, analyze, and realize complex mechanical metamaterials with novel functionalities; We employ combinatorial strategies to construct metamaterials that can deform to arbitrary numbers of pre-defined textures.

We use topological defects to steer deformations and stresses towards desired parts of the system. We construct topologically non-trivial knots and links in the defect pattern or in the deformation field.

We use the degenerate and disordered manifold of mechanically stable states to detect the sequence of operations that a material underwent.

Abstracts

Erika Tsingos

Utrecht University, The Netherlands

COMPUTATIONAL MODELLING OF ANIMAL DEVELOPMENT

Animal development is fascinatingly complex.

At the subcellular level, an intricate machinery of thousands of molecular components churns. It ensures that the right genes are expressed at the right time and place, and shapes cells from the inside to give rise to specialized structures such as nutrient-absorbing protrusions.

At the cell level, relatively few behaviours emerge such as cell division, migration, and cell-cell adhesion. Acting as a collective, cells give shape to organs and maintain them lifelong by constantly repairing wear and tear.

These scales – subcellular, cellular, and organ-scale – are not isolated, but cross-regulate by feedback interactions. Computational models are perfectly poised to disentangle such complex relationships by isolating the contributions of each factor, both testing and generating new hypotheses.

In my talk, I will give an overview of the field of cell-based computational models and highlight examples of new model developments in my research group.

Speakers'

Monday, March 23
9:05 AM–9:45 AM

Martin Wegener

Karlsruhe Institute of Technology (KIT), Germany

DESIGNING MANUFACTURABLE 3D METAMATERIALS

Metamaterials are rationally designed composites allowing for effective-medium properties that go qualitatively or quantitatively beyond ('meta') those of the bulk ingredients [1]. Many metamaterials can and have been made by means of 3D printing [2], and can in turn by viewed as 'meta-inks' for 3D printing. In many instances [1,3], the properties of a composite made of ingredient materials A and B are not in between those of A and B. In interesting cases, the properties lye outside the interval defined by A and B. Sometimes, the properties can even be negative with respect to those of A and B [1]. Sometimes, the properties are even unbounded [1].

Metamaterials cover the entire breadth of solid-state-physics, ranging from electromagnetic and optical properties, to static and dynamic elastic, acoustic, as well as charge-, mass-, and energy-transport properties.

Designing a metamaterial poses an inverse problem: One targets certain effective properties and searches for a manufacturable 3D microstructure that that exhibits these properties. For us, this process has always involved human intelligence.

In this talk, I present selected examples of our past work [1] and of our more recent work [3]. The latter focuses on nonlocal wave and diffusion properties, engineered by beyond-nearest-neighbor inter-actions in periodic lattices (crystals) [3].

[1] "3D Metamaterials", M. Kadic, G.W. Milton, M. van Hecke, and M. Wegener, Nature Rev. Phys. 1, 198 (2019)
[2] "The physics of 3D printing with light", P. Somers, A. Münchinger, S. Maruo, C. Moser, X. Xu, and M. Wegener, Nature Rev. Phys. 6, 99 (2024)
[3] "Nonlocal metamaterials and metasurfaces", Y. Chen, R. Fleury, P. Seppecher, G. Hu, and M. Wegener, Nature Rev. Phys. 7, 299 (2025)

Abstracts

Tanja Weil

Max Planck Institute for Polymer Research, Mainz, Germany

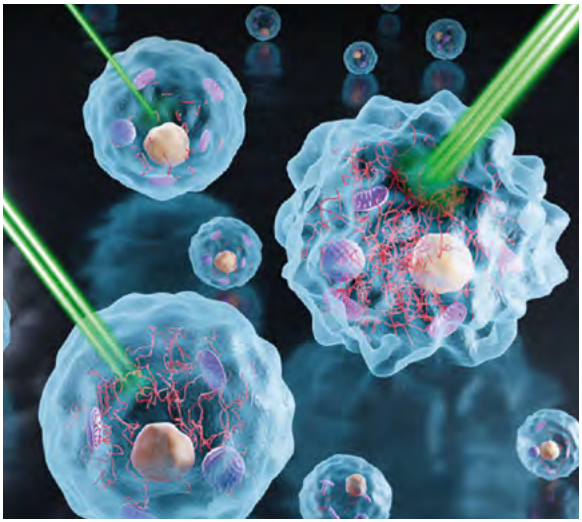
SUPRAMOLECULAR DESIGN PRINCIPLES FOR MATERIAL–CELL COMMUNICATION

We present synthetic supramolecular systems that form and operate within living environments to control cellular function. Our in-cell synthesis strategy uses endogenous redox, enzymatic, and metabolic inputs or light to trigger supramolecular assembly and catalytic activity, enabling state-dependent modulation of mitochondrial metabolism and immune function.

In parallel, we design artificial cells with chemically encoded sensing and actuation capabilities that exchange metabolites with natural cells, forming hybrid systems with bidirectional communication.

These approaches establish a materials-based route to influence cellular fate without genetic manipulation and provide design principles for autonomous therapeutic systems and synthetic organelles.

Figure 1: Bioresponsive caged peptide monomers enter living cells and undergo chemical transformations initiated by light and form supramolecular peptide nanofibers that can control cellular processes (Y. Ren et al. Nature Synthesis 2025).



Contributed Talks

Sorted by Date

MONDAY, MARCH 23

10:40 AM–11:55 AM	Dynamic Control of Rigidity Via Geometric Frustration in Stimuli-Responsive Mechanical Metamaterials	**Santiago Gomez Melo**
10:55 AM–11:10 AM	Geometry Screening of A 3D-Printed Biocatalytic Reactor	**Bruno Vuillod**

TUESDAY, MARCH 24

11:15 AM–11:30 AM	Multiscale Modelling of The Linear and Nonlinear Optical Response Of Molecular Materials And Devices Thereof	**Marjan Krstić**
11:30 AM–11:45 AM	Design Optimization of Printed Thermoelectric Generators for Energy Harvesting and Waste Heat Recovery	**Muhammad Irfan Khan**
11:45 AM–12:00 PM	Structural Flexibility Explains Solvent-Induced Spectral Shift in Styrylpyrene	**Samira Gholami**

WEDNESDAY, MARCH 25

1:30 PM–1:45 PM	Deep Learning-Based Inverse Design of Holographically Produced 3D Photonic Metamaterials with Tailored Photon Density of States	**Zesen Zhou**

A Contributed Talk consists of a 10-minute talk and a 5-minute Q & A session.

Monday, March 23
10:40 AM–11:55 AM

DYNAMIC CONTROL OF RIGIDITY VIA GEOMETRIC FRUSTRATION IN STIMULI-RESPONSIVE MECHANICAL METAMATERIALS

Santiago Gomez Melo

Santiago Gomez Melo [1,2], Falko Ziebert [1,2], Ulrich S. Schwarz [1,2]

1: Institute for Theoretical Physics, Heidelberg, Germany
2: BioQuant, Heidelberg, Germany

Recent advances in materials design and 4D-printing now allow one to realize programmable metamaterials that upon receiving a suitable stimulus dynamically change their unconventional macroscopic properties.

For mechanical metamaterial, these tunable features have so far been restricted to geometric quantities, such as the Poisson ratio and the strain-to-twist ratio, but the effective elastic moduli have not been addressed yet.

Here we combine central force network theory and responsive hyperelasticity to show that it is also possible to dynamically control the elastic moduli, and more specifically the shear modulus, by programming geometric frustration into a stimuli-responsive structure. This phenomenon, known as geometric incompatibility, produces a rigidity phase transition in which the elastic modulus changes by several orders of magnitude. It results from inducing a state of self-stress that eliminates the floppy modes of the system by producing second-order rigidity.

The underlying physical principle seems to be also at work in biological systems, most prominently in epithelial monolayers, but here it is predicted for entirely synthetic materials, like temperature-sensitive hydrogels and nematic elastomers, opening up the perspective of designing a new class of dynamic metamaterials.

GEOMETRY SCREENING OF A 3D-PRINTED BIOCATALYTIC REACTOR

Bruno Vuillod

Bruno Vuillod, Anca Pordea, Simon Attwood, Jordan Hill, Mirco Magnini, Ricky Wildman

Faculty of Engineering, University of Nottingham, Nottingham, United Kingdom

Additive manufacturing enables the fabrication of increasingly sophisticated geometries, opening new possibilities for the design of functional reactors. In contrast, pharmaceutical processes involving enzymatic reactions are often inefficient: once used, enzymes are generally difficult, costly, or even impossible to recover for reuse. One promising strategy is to embed enzymes directly within the volume of a hydrogel microreactor, allowing their use in continuous production processes. However, enzyme immobilisation typically leads to a significant reduction in catalytic efficiency, mainly due to transport limitations.

Following a preliminary proof-of-concept [1] and the development of a dedicated printable hydrogel material, the next challenge is to exploit geometric design to enhance mass transfer and increase the overall production rate. The current reactor architecture consists of a straight channel operating under laminar flow conditions, in which a large fraction of the inlet substrate remains confined to the channel core and does not effectively reach the enzyme-loaded hydrogel.

The objective of this work is to improve reactor performance through geometric enhancement enabled by additive manufacturing. Starting from the straight channel, multiple lattice-based geometries are designed and screened using numerical simulations of coupled fluid flow and mass transport.

The impact of key geometric descriptors —such as global and local residence time, surface-area-to-volume ratio, and tortuosity — is analysed to assess their role in promoting substrate transport toward the reactive regions.

[1] Attwood, S. J., Leech, D., He, Y., Croft, A. K., Hague, R. J. M., Irvine, D. J., Wildman, R. D., & Pordea, A. (2025). High resolution 3D printed biocatalytic reactor core with optimized efficiency for continuous flow synthesis. Chemical Engineering Science, 305. https://doi.org/10.1016/j.ces.2024.121156

MULTISCALE MODELLING OF THE LINEAR AND NONLINEAR OPTICAL RESPONSE OF MOLECULAR MATERIALS AND DEVICES THEREOF

Marjan Krstić

Marjan Krstić [1], Mariia Poleva [1], Christof Holzer [1,2], Ivan Fernandez-Corbaton [3], Carsten Rockstuhl [1,3,4]

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2: Institute of Quantum Materials and Technologies, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
3: Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
4: Center for Integrated Quantum Science and Technology, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Modeling light-matter interactions in extended systems, such as crystalline molecular films or supramolecular assemblies containing millions of atoms, presents significant theoretical challenges. Describing such systems correctly requires bridging the gap between atomic-scale quantum chemistry simulations and electromagnetic response at the level of the entire material. To achieve this, we have developed a multiscale framework combining precise electronic structure calculations with efficient electromagnetic scattering simulations.

Our interdisciplinary scale-bridging multi-scattering framework [1,2] enables us to investigate linear and nonlinear optical responses in systems that far exceed the capabilities of traditional quantum chemistry. The framework allows us to unravel complex light-matter interactions by understanding the fundamental origins of the photo-physical properties of a given molecular material. At the same time, we can incorporate those materials in a complex multi-material photonic environment to design advanced optical devices. In a bottom-up approach we compute both the dynamic polarizabilities and the first hyperpolarizabilities of the building blocks of the material at the quantum level and convert them to a T-matrix and a hyper-T-matrix to express the linear and the nonlinear response in multi-scattering simulations.

To overcome current challenges on the quantum level, we further extended the calculations to the time domain and incorporated a sum-over-states approach. Such an approach facilitates studies of solid-state materials like silicon and metal-organic frameworks, as well as their complex nonlinear response, such as magnetically dependent chiral second-harmonic generation. These extensions pave the way for the rational design of optical devices with properties tailored on demand. Preliminary results, along with a discussion of current theoretical challenges, will be presented.

[1] B. Zerulla, M. Krstić, D. Beutel, C. Holzer, C. Wöll, C. Rockstuhl, I. Fernandez-Corbaton, Adv. Mater., 34, 2200350, (2022)
[2] B. Zerulla, D. Beutel, C. Holzer, I. Fernandez-Corbaton, C. Rockstuhl, M. Krstić, Adv. Mater., 36, 2311405, (2024)

DESIGN OPTIMIZATION OF PRINTED THERMOELECTRIC GENERATORS FOR ENERGY HARVESTING AND WASTE HEAT RECOVERY

Muhammad Irfan Khan

Muhammad Irfan Khan[1], Zirui Wang[1], Nan Luo[1], Leonard Franke[1,2], Md. Mofasser Mallick[1,2], Uli Lemmer[1,3,4]

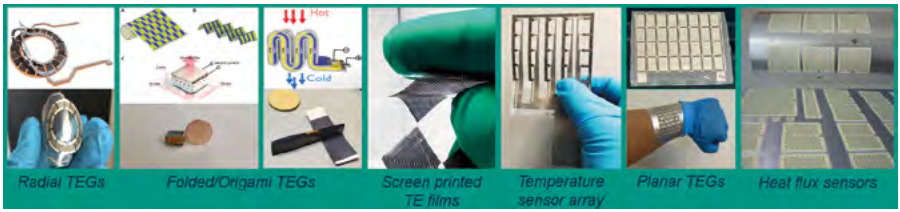
1: Light Technology Institute, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany
2: Varmo UG, Karlsruhe, Germany
3: InnovationLab GmbH, Heidelberg, Germany
4: Institute of Microstructure Technology, Karlsruhe Institute of Technology (KIT), Eggenstein-Leopoldshafen, Germany

Recently, thermoelectric generators (TEGs) have gained significant attention for directly converting waste heat into electricity. Due to the considerable variations in heat-source and sink geometries and boundary conditions, the design of TEGs should offer flexibility to fulfill the specific constraints. Printing technologies, such as screen printing or 3D printing, offer versatile, cost-effective manufacturing approaches for TEGs, enabling scalability and shape conformability.

However, developing high-performance fully printed TEGs is not straightforward and requires extensive optimization of printed material and device design. In this work, we present essential theory and computations for the design and optimization of printed TEGs to achieve maximum power output under specified boundary conditions.

We designed and analyzed several TEG layouts and structures (e.g., planar, radial, and origami) for a range of applications, from low-power electronics and autonomous systems to large-scale waste heat recovery. The general criteria for simultaneous thermal and electrical impedance optimization must be fulfilled to ensure optimal performance of the TEG system for any application.

This can be achieved primarily by adjusting the TEG fill factor, leg dimension, and the cross-sectional areas of the n-type and p-type legs. This printing of TEGs, along with computational optimization techniques, significantly reduces the cost per watt (€/W) and LCOE (€/kWh) for these applications.



STRUCTURAL FLEXIBILITY EXPLAINS SOLVENT-INDUCED SPECTRAL SHIFT IN STYRYLPYRENE

Samira Gholami

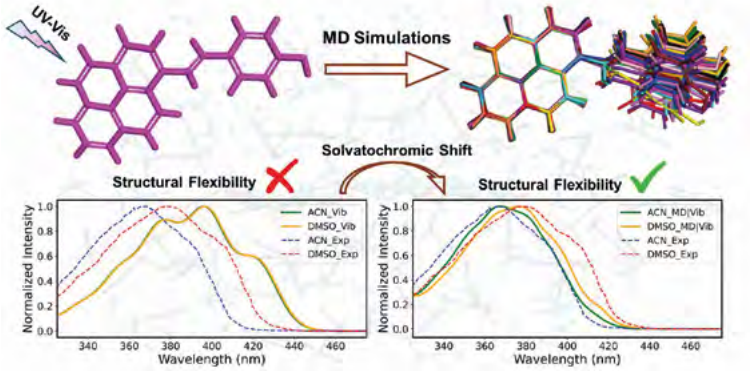
Samira Gholami , Anna Mauri, Wolfgang Wenzel, Mariana Kozlowska

Institute of Nanotechnology, Karlsruhe Institute of Technology (KIT),Karlsruhe, Germany

Understanding solvent-induced spectral tuning and its connection to photochemical reactivity remains a challenge for photoactive molecular systems. In styrylpyrene, a chromophore involved in light-driven [2+2] cycloaddition, experimental solvatochromic shifts have long lacked a consistent theoretical explanation, hindering predictive modeling of its reactivity.

Here, we combine quantum-mechanical (QM) calculations with molecular dynamics (MD) sampling within a multiscale computational strategy to resolve the microscopic origins of these solvent effects. The findings, highlighting the limitation of traditional static approaches in predicting the absorption spectral line-shape and its solvent dependence, reveal a cooperative interplay between conformational flexibility, solvent-modulated electrostatic polarization, and vibronic coupling that contributes mostly in determining the solvent-induced spectroscopy of this molecule.

By employing ensemble-based electronic-structure calculations integrated with vibronic approaches, we accurately reproduce the experimentally observed red-shift in polar solvents such as acetonitrile and dimethyl sulfoxide. The resulting framework provides a methodological guideline for reliably simulating flexible chromophores and enables the rational design of photo-programmable molecules and materials with tailored optical and reactive properties, thereby improving control over light-triggered processes in complex environments.



DEEP LEARNING-BASED INVERSE DESIGN OF HOLOGRAPHICALLY PRODUCED 3D PHOTONIC METAMATERIALS WITH TAILORED PHOTON DENSITY OF STATES

Zesen Zhou

Faculty of Science /Department of Physics, Lund University, Sweden

Three-dimensional (3D) photonic metamaterials enable efficient control of light-matter interactions through engineering of the photon density of states (pDOS). While metasurface-based holographic lithography provides a scalable route for fabricating corresponding 3D photonic structures, designing the metasurface patterns required to realize tailored pDOS distributions remains a nontrivial challenge.

Here, we propose a generative learning-based inverse design framework that directly links target pDOS peaks to fabrication-ready metasurface patterns for holographic lithography. The framework employs a generative adversarial network (GAN) to generate target diffraction orders and lithography exposure thresholds for achieving tailored pDOS features, followed by a particle swarm optimization-FDTD cooptimization to retrieve metasurface patterns corresponding to these targets.

With this framework, we achieved inverse design of a metasurface that realizes a 3D photonic metamaterial with pronounced local pDOS enhancement at a prescribed normalized frequency of 0.5. The normalized pDOS reaches a peak of about 3.93, corresponding to nearly a fourfold increase relative to an effective homogeneous-material reference. The 3D morphology exhibits a characteristic rotational symmetry within the unit cell, with the upper half symmetric along the *x* direction and the lower half symmetric along the *y* direction connected through a central region corresponding to a 90° rotation. Extending the inverse design across normalized frequencies from 0.45 to 0.7 reveals that 3D structures sharing this structural motif consistently exhibit localized pDOS enhancement.

Overall, this work provides a practical inverse design approach that can be readily applied to future holographic lithography for 3D photonic metamaterials.

Flash Talks & Poster Presentation

Monday, March 23

Flashtalks
5:00 – 5:10 PM

Poster Session I
5:10 – 6:00 PM

Wednesday, March 25

Flashtalks
3:20 – 3:30 PM

Poster Session II
3:30 – 4:20 PM

A Flashtalk is a short, 60-second presentation.
Everyone who gives a Flashtalk gives a Poster Presentation as well.

Flashtalks & Poster Presentation

Monday, March 23 | Flashtalks: 5:00 – 5:10 PM | Poster Session I: 5:10 – 6:00 PM	
Single-SHOT Volumetric Additive Manufacturing via Computer Generated Holograms	**Junhee Lee**
3D Laser Printing for Controlling Heart Organoid Models	**Tamara Unterreiner**
3D Multiphoton Laser Printing of Block Copolymers for Hierarchically Nano-Ordered Architectures	**Moritz Philipp Hopp**
Theory-Guided Design of Push-Pull Chromophores for Silicon-Organic Hybrid Modulators	**Fritz Henke**
4D Microprinting of Dual-Shape and Triple-Shape Memory Polymers	**Lilliana Flórido Martins**
Field-Effect Transistors Used for Biological Applications	**Merve Nur Ekmekci**
Cellular Contraction Forces In 3D Hydrogel Scaffolds Fabricated by Two-Photon Direct Laser Writing	**Kathi Michèle Kaiser**
Electron Energy Loss Fine Structure Analysis of Metallic Glasses	**Arne Johan Schwartz**
In Situ Bioprinting of Patterned Corneal Tissue Constructs	**Mario Wisbar**
Rapid 3D Fabrication with Dynamic Holographic Sound Fields	**Julius Dehne**
Printed High-Entropy MOF for Non-Volatile Memristive Devices	**Yan Liu**
Constrained Shape Optimisation of Milling Geometries to Minimise Thermal Stresses in Lamella for Cryo-Em	**Cornelis Mense**
Oblique Plane Microscopy with Metasurfaces	**Maryna Meretska**
Spatially Nonlocal Metamaterials for Tailored Anomalous Diffusion	**Ke Wang**

Wednesday, March 25 | Flashtalks: 3:20 – 3:30 PM | Poster Session II: 3:30 – 4:20 PM	
Insight Into the Poling Behavior of Monolithic Electrooptic Materials	**Philipp Dullinger**
Modulating Two-Photon Absorption in a Pyrene-based MOF series: Structure-Property Relationships	**Helmy Pacheco Hernández**
An Automated Workflow for Predicting First Hyperpolarizabilities of Donor-Acceptor Chromophores for NLO Devices	**Jia Gao**
A Series of Printable Group 14 Chalcogenide Clusters with Optical Multifunctionality	**Jie Wang**
Enhancing Triplet Excitons Lifetime Through Controlled Intermolecular Interactions	**Martin Richter**
Development and Understanding of Enantioselective Passerini Three Component Reaction	**Sonia Sonia**
Applying Machine Learning to Predict Photochemical Action Plots and Wavelength Dependent Quantum Yields	**Magdalena Unterreiner**
Beyond Norrish-Type Reactivity: A Novel Photoinitiation Mechanism for Biacetyl in Two-Step Two-Colour 3D Microprinting	**Vitalii Shekhovtsev**
Inverse Design and Optimization of a Photonic Coupler	**Julius Paul Schmieta**
Towards A Fully Differentiable Digital Twin for Solar Cells	**Marie Louise Schubert**
From Molecules to Metasurfaces: Fast Multiscale Modeling of Thermal Emission	**Martin Gabbert**
T-Matrix-Based Multiple-Scattering Modeling of Acoustic Metamaterials and Metasurfaces	**Nikita Ustimenko**
Applications of a Multiscale Framework for Nonlinear Optical Simulations in Periodic Structures	**Mariia Poleva**
Inverse Design of 3D Nanophotonic Devices	**Oliver Kuster**

SINGLE-SHOT VOLUMETRIC ADDITIVE MANUFACTURING VIA COMPUTER GENERATED HOLOGRAMS

Junhee Lee

Junhee Lee[1,2], Lovish Gulati[1,2], Alexander Song[1,2], Kai Melde[1,2], Peer Fischer[1,2,3,4]

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We introduce a fabrication approach based on holographic microlithography that produces three-dimensional microstructures in a single exposure. A spatial lightmodulator is used to tailor coherent illumination into a 3D intensity distribution, enabling the entire object to be polymerized as one piece during a short exposure ofroughly 10 ms. Phase masks are computationally designed for specific target geometries using computer-generated holography (CGH). In particular, we use the Non-Convex Optimization for Volumetric CGH (NOVO-CGH) algorithm [1], which offers good reproducibility, reduced speckles, and high contrast between illuminated regions and the dark background, thereby confining photopolymerization to the intended volumes. Polymerization occurs primarily in bright regions where the delivered dose surpasses a photopolymerization threshold.

We apply this method to fabricate three-dimensional soft microactuators from liquid-crystal (LC) elastomers. Because the 3D light pattern triggers UV curing throughout the LC structure almost simultaneously, it maintains molecular alignment during polymerization[2] while allowing the complete 3D architecture to be defined in a single exposure step.

As a result, molecular orientation can be tuned independently of actuator geometry — capabilities that conventional fabrication approaches cannot achieve[3].

[1]J.Zhang et al., 3D computer-generated holography by non-convex optimization, Optica, 4(10), 1306-1313 (2017)
[2]L.Gulati et al., Aligning and Observing the Liquid Crystal Director in 3D Using Small Magnetic Fields and a Wedge-Cell, Advanced Functional Materials, 35(3),2413513 (2024)
[3] L.Gulati, J.Lee Holographic Whole-Object Photopolymerization Preserving Director Alignment in Liquid Crystalline, submitted.

3D LASER PRINTING FOR CONTROLLING HEART ORGANOID MODELS

Tamara Unterreiner

Tamara Unterreiner[1], Annika Vogler[2], Paolo Chiarandà[1], Eileen Furlong[2], Christine Selhuber-Unkel[1]

1: Institute for Molecular Systems Engineering and Advanced Materials (IMSEAM), University Heidelberg, Germany
2: European Molecular Biology Laboratory (EMBL), Heidelberg, Germany

Cardiovascular disease remains a leading cause of global mortality, with many adult-onset cardiomyopathies tracing back to developmental origins. Despite this, the mechanisms underlying human heart development and disease progression remain poorly understood due to the limitations of existing model systems. Human heart organoids (hHOs), derived from human induced pluripotent stem cells (hiPSCs), represent a transformative model for studying early cardiogenesis and patient-specificgenetic disorders. However, current hHO models are hindered by low complexity, significant morphological heterogeneity, and poor reproducibility — particularly in terms of shape and internal organization.

This project aims to overcome these limitations by developing advanced bioengineering strategies to direct and standardize heart organoid morphogenesis. A materials-based approach is employed, utilizing 3D printed scaffolds with tailored mechanical and structural properties to guide tissue organization during hHO development. A range of biomaterials, primarily hydrogels and elastomeric compounds, are systematically varied in stiffness, porosity, and topography to mimic the biomechanical environment of early heart tissue and to promote the formation of multichambered heart structures with reduced variability.

Through the combination of additive manufacturing, materials science, and bioengineering, this project aims to provide a robust framework for the directed development of cardiac organoids. The underlying strategies are expected to be broadly transferable to other organoid systems, offering a new paradigm for engineering complex tissue models with high fidelity and consistency.

3D MULTIPHOTON LASER PRINTING OF BLOCK COPOLYMERS FOR HIERARCHICALLY NANO-ORDERED ARCHITECTURES

Moritz Philipp Hopp

Moritz Philipp Hopp[1], Nadine von Coelln[2], Santiago Gomez Melo[3], Petra Tegeder[2], Ulrich S. Schwarz[3,4], Eva Blasco[1]

1: IMSEAM, Heidelberg University, Germany
2: Physikalisch-Chemisches Institut, Heidelberg University, Germany
3: Institute for Theoretical Physics, Heidelberg University, Germany
4: Bioquant-Center, Heidelberg University, Germany

Block copolymers (BCPs) are comprised of two or more connected blocks of chemically distinct monomer units. Employing controlled radical polymerization methods, such as reversible addition fragmentation chain transfer (RAFT), atom-transfer radical polymerization (ATRP), or nitroxide-mediated polymerization (NMP), enable facile and straight-forward synthetic access to BCPs, while control over polymer characteristics like molecular weight, dispersity, and the sequence of incorporated monomers is maintained.

The arising segmented structure of BCPs imparts this class of polymer architecture with the unique ability to spontaneously self-assemble into nanoscale morphologies with precise order, integral for applications such as membranes, biomedical devices, or semiconductors. Depending on the chemical composition of the BCP and the interactions energies between the blocks, theoretical calculations predicted the self-assembly process to form diverse morphologies, including spheres, cylinders, and lamella, in agreement with experiments. In order to obtain functional, hierarchical ordered materials based on BCPs, multi-photon laser polymerization (MPLP) has proven to be a useful tool for fabricating hierarchically ordered microstructures with arbitrary geometries. Hereby, computer simulations can help to guide experiments, including finite size and kinetic effects that arise during the printing process.

However, the current material scope for fabricating self-assembled 3D structures with MPLP is limited and largely unexplored. Herein, new inks for MPLP based on BCPs are formulated, printed, and investigated in terms of their self-assembling behavior. By carefully tuning the molecular composition of the synthesized BCPs, distinct morphologies were obtained and characterized. Implementing the self-assemblies into inks, suitable for MPLP, resulted in microstructures of desired geometries with well-defined morphologies on the nanoscale. By implementing this bottom-up approach, the presented work highlights the potential of combining molecular design to govern self-assembly on the nanoscale with MPLP, establishing structured micromaterials.

THEORY-GUIDED DESIGN OF PUSH-PULL CHROMOPHORES FOR SILICON-ORGANIC HYBRID MODULATORS

Fritz Henke

Fritz Henke[1,2], Maximilian Hartmann[2], Masis Sirim[1,2], Patrick Kern[1,2], Sidra Sarwar[1,2], Philipp Dullinger[3], Celso Ricardo Caldeira Rego[3], Peter Erk[4], Christian Koos[4,5], Wolfgang Wenzel[3], Stefan Bräse[1,2]

1: Institute of Organic Chemistry (IOC)
2: Institute of Biological and Chemical Systems -Functional Molecular Systems (IBCS-FMS)
3: Institute of Nanotechnology (INT)
4: Institute of Photonics and Quantum Electronics (IPQ)
5: Institute of Microstructure Technology (IMT)

all at Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

The rapid expansion of artificial intelligence, cloud computing, and emerging quantum technologies has driven an unprecedented increase in global data traffic and energy consumption. Addressing this challenge requires faster and more energy-efficient data transmission technologies. Photonic integrated circuits (PICs) offer a promising route by enabling high-bandwidth, low-loss optical data transfer. Modulators are one of the key components within PICs to convert electrical signals intooptical signals.

Silicon-organic hybrid (SOH) modulators are particularly attractive as they combine the scalability of silicon photonics with the exceptional performance and tunability of organic electro-optic (OEO) materials. These materials are based on push-pull chromophores, whose large molecular dipole moments and hyperpolarizabilities give rise to EO coefficients exceeding those of conventional inorganic materials. State-of-the-art CLD-type chromophores face an inherent trade-off between high molecular hyperpolarizability and increased optical loss due to absorption at telecommunication wavelengths, as well as limitations in photo- and thermal stability.

To overcome these challenges, we employ a theory-guided chromophore design strategy using an automated density-functional theory (DFT) workflow. The DELFIN framework enables prediction of dipole moments, hyperpolarizabilities, and electronic excitations, from SMILES input through global conformer exploration to high-level DFT calculations in ORCA. Benchmarking against literature chromophores shows good agreement with experimental hyper-Rayleigh scattering and absorbance data.

Future developments will focus on the evolutionary design of novel chromophores using automated, deep-learning-driven molecular morphing, combined with multiscale modeling of chromophore alignment in thin films. This integrated discovery funnel aims to identify promising candidates prior to time-consuming chemical synthesis, accelerating the development of next-generation OEO materials for energy-efficient SOH modulators.

4D MICROPRINTING OF DUAL-SHAPE AND TRIPLE-SHAPE MEMORY POLYMERS

Lilliana Flórido Martins

Lilliana Flórido Martins[1,2], Christoph A. Spiegel[1,2], Eva Blasco[1,2]

1: Institute for Molecular Systems Engineering and Advanced Materials, Heidelberg University, Germany
2: Instituteof Organic Chemistry, Heidelberg University, Germany

Shape memory polymers (SMPs) are a promising class of smart materials that can recover from a programmed shape to their original one when exposed to suitable stimuli, making them highly attractive for biomedical applications, aerospace engineering and soft robotics. To shape such materials, 4D printing has emerged for the fabrication of responsive 3D structures, implementing time as a fourth dimension via smart responsive materials. While 4D printing of SMPs is well studied in macroscale systems, microscale printing is less explored: Up to now, all 4D microprintable SMPs are based on glass transitions and limited to a dual-shape memory effect (SME) allowing only one programmable shape, thus lacking options for more complex actuation required for advanced soft microrobotics.

To address this gap, we present an approach based on two semicrystalline polylactone prepolymers targeting dual- and triple-SMP ink formulations for multiphoton 3D laser printing. Following prepolymer synthesis and functionalization with photopolymerizable groups, two ink formulations are established for a dual- and triple-SME respectively. For both, printing conditions are carefully evaluated, affording complex geometries with intricate details and high shape fidelity. After characterizing the thermal transitions of the underlying network, shape memory protocols are established. Both dual- and triple-shape memory microstructures show stable shape fixation in programmed states along with repeatedly full recovery to the printed, permanent shape. While the dual-shape memory structures recover in one step, the triple-shape memory structures show stepwise recovery via a stable partly recovered shape. By leveraging the properties of semicrystalline SMPs, our systems achievefinely tunable, stepwise responses and controlled actuation at the microscale, paving the way for advanced soft microrobotics and adaptive miniature devices.

FIELD-EFFECT TRANSISTORS USED FOR BIOLOGICAL APPLICATIONS

Merve Nur Ekmekci

Karlsruhe Institute of Technology, Germany

Cancer is a disease with one of the highest mortality rates. Despite significant advancements in modern science and medicine, cancer is still challenging to treat. To preserve tissue homeostasis, cells go through strictly controlled processes of growth, division, and programmed death. Therefore, it is crucial to detect cancerous cells at an early stage.

The BioFETs consist of ITO drain and source electrodes as well as inkjet-printed In_2O_3 as the channel. Subsequently, biotinylated lipid membranes are patterned viacapillary printing on the channel. For electrical characterization, phosphate-buffered saline and a composite solid polymer electrolyte are constrained in the channel area of the BioFET. Finally, bovine serum albumin and streptavidin layers are sequentially applied via pipetting.

In the In_2O_3 liquid-gated device, PBS deposition caused a negative shift in threshold voltage, due to electric double layer formation and strong ionic gating. In the absence of lipids, the threshold voltage shifted to more negative values. This shift is indicative of enhanced gate coupling and a more stabilized electrolyte/semiconductor interface. However, when a lipid layer was present, PBS produced a strong degradation in subthreshold behavior together with a pronounced negative shift of the threshold voltage, suggesting reduced effective gate capacitance and increased interfacial polarization/ trapping. After BSA blocking, the threshold voltage only showed a minor shift toward more positive values in both lipid and no-lipid cases. Finally, streptavidin adsorption resulted in a small additional positive shift of the threshold voltage for both conditions, indicating biomolecular-induced interfacial charge/dipole effects and enhanced trapping or polarization dynamics.

In future works, the sensing ability of the BioFET/EGFET device will be further characterized by immobilizing certain biorecognition probe molecules, such as antibodies, and then exposing the sensors to cancer-related protein biomarkers. The variations in the transfer curve parameters, such as Vth changes, subthreshold slope, and hysteresis, will be monitored and analyzed to confirm the sensing and binding effects.

CELLULAR CONTRACTION FORCES IN 3D HYDROGEL SCAFFOLDS FABRICATED BY TWO-PHOTON DIRECT LASER WRITING

Kathi Michèle Kaiser

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Contractile forces play a crucial role in numerous cellular processes. Although cells *in vivo* are embedded in a three-dimensional environment, most *in vitro* studies are performed in two-dimensional systems. To accurately investigate cellular contractility and how we can influence them, well-defined three-dimensional environments are essential.

This requires a material with tuneable stiffness and adhesiveness as well as flexible geometries enabling the investigation of cellular forces in different 3D settings. To accomplish this task, we employed Two-Photon Direct Laser Writing to fabricate custom-designed 3D scaffolds. For this purpose, we developed our own hydrogel-based printing material, poly(acrylamide-co-acrylic acid) (pAm_AA).

Using this ink, it is possible to print complex 3D structures that remain stable for several months. Also, the material is biocompatible and can be biofunctionalized to support adhesion of different cell types.

With 3D Traction Force Microscopy, cellular contraction forces can be quantified by analysing scaffold deformations induced by the cells. This method enables the investigation of the cellular forces depending on environmental architecture and stiffness.

To investigate cellular forces, we are using two different cell types so far, fibroblasts as a reference cell type and cardiomyocytes as a highly contractile muscle cell model. Both cell types effectively deform the hydrogel scaffolds, yielding promising measurements of contraction forces.

ELECTRON ENERGY LOSS FINE STRUCTURE ANALYSIS OF METALLIC GLASSES

Arne Johan Schwartz

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Introduction: Many technologically relevant materials are amorphous, including polymers, oxides and glasses. PdNiP metallic glasses exhibit exceptional mechanical properties combined with excellent glass forming ability making them an excellent model system. Extended electron energy loss fine structure (EXELFS), the electron-based analogue of XAFS, provides element-resolved information on short-range order (SRO). Compared to XAFS, EXELFS enables correlation with other powerful transmission electron microscopy (TEM) techniques. In this work, EXELFS is applied to metallic glasses with different compositions to investigate structural differences in their local atomic order, after validation on model systems and systematic optimization of experimental parameters.

Methods: The EXELFS signal is simulated with varying parameters to assess their influence on data quality and analysis reliability. As a model system, EXELFS measurements were performed on a polycrystalline aluminum sample. EXELFS measurements were carried out on PdNiP samples. The achieved data quality is limiting the confidence in the evaluated physical parameters. Further optimization for the data acquisition is suggested.

Results: The extracted partial pseudo-radial distribution function of the aluminum model system shows agreement with simulations. To judge the quality of the EXELFS analysis, electron diffraction data will be recorded. For the metallic glass samples, limitations in signal quality and challenges in data analysis were determined. To improve a reliable extraction of elemental-resolved SRO, the signal-to-noise ratio and other crucial parameters are studied.

Discussion and Conclusions: The promising results obtained for the aluminum sample show the overall viability of this technique. The accuracy of the EXELFS data is limited by the signal-to-noise ratio, the evaluated energy range and a scattering phase shift. In contrast, the more complex structure in metallic glasses introduces additional experimental and analytical challenges, that need more sophisticated analysis steps to obtain accurate and reliable results.

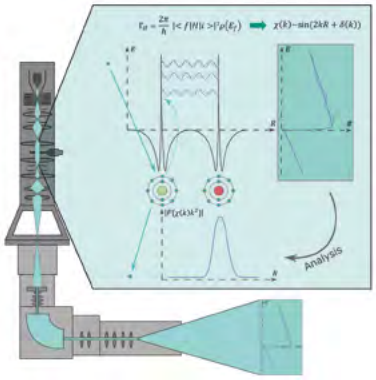

Fig. 1: Schematic of EXELFS signal formation. Scattering of the outgoing spherical wave produced by inelastic electron scattering gives rise to oscillations in the fine structure. After background subtraction and Fourier transformation, a partial pseudo-radial distribution function is obtained, providing nearest-neighbor distances and coordination numbers.

IN SITU BIOPRINTING OF PATTERNED CORNEAL TISSUE CONSTRUCTS

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Aim and Objective: Human tissues show complex architecture beyond the visible level, which is highly important for their function. A prime example is the human cornea, the major refractive lens of the eye, where structural integrity is vital for force distribution and especially its transparency. We are dedicated to advance the in situ restoration of the human cornea by bioprinting the tissue directly onto the patient's eye and aim to combine bioprinting with acoustophoresis to recreate the microstructure of the cornea for increased transparency and structural integrity.

Materials and Methods: Human bone marrow mesenchymal stem cells were patterned into parallel stripes using ultrasound. The patterns were analyzed by Voronoi tessellation and kept in culture to observe their further growth, migration and cell alignment, which facilitates directional matrix remodeling. This study focusses on a novel approach to guide ultrasound to the printing site for the undistorted transmission of the sound in situ, which is critical for the integration of acoustophoresis into bioprinting.

Results: Patterning was successfully achieved in 2D cultures as well as on gelatine dummies of the human eye. Ex vivo tests on pig eyes are preliminary. Patterned cells started to grow perpendicular from the stripes and alignment was observed after two weeks in culture. Prototypes of the transducer were tested for 1 MHz and 4.8MHz, comparing quality and quantity of the patterns.

Conclusions: While patterning cells with acoustophoresis is rising in tissue engineering, its in situ application and integration into bioprinting processes is challenging. We present strategies to overcome this challenge and especially focus on the design process involved.

RAPID 3D FABRICATION WITH DYNAMIC HOLOGRAPHIC SOUND FIELDS

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Acoustic radiation forces offer a promising approach for remote, contactless particle manipulation. Using holographic methods and 3D-printed phase plates, it was shown that ultrasound fields can assemble microparticles at a distance into connected 2D structures. Since sound waves are non-ionizing mechanical waves, they propagate deep into biological tissues and are cytocompatible at low excitation amplitudes, making them an emerging tool in biofabrication and biomedical stimulation.Recently, the first 3D assembly of whole objects in a single exposure using compact holographic ultrasound fields from multiple sources was demonstrated, highlighting potential tissue engineering applications.

Due to coherent, single-frequency excitation, interference effects produce periodic discontinuities in the trapping regions. The project explores strategies to assemblefully connected 3D structures in a single shot. This involves exploiting the inertia of microparticles and cells and a dynamically tuned radiation force potential in 3D. One approach is to phase-modulate one of the individual transducers to create effective continuous traps. Another approach is to use multiple sources (starting with 16 or 32), each driven separately by a multichannel amplifier at potentially different frequencies.

For this, the computational tools will be expanded to include time-resolved radiation force calculations. Additionally, the results from phase and frequency modulation are used in the optimization code to improve the computer-generated holograms.

As an additional part of the project, we want to explore acoustic metamaterials to improve the efficiency of holograms by modulating the amplitude as well as the phase and exhibiting high sound transmission.

PRINTED HIGH-ENTROPY MOF FOR NON-VOLATILE MEMRISTIVE DEVICES

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As fundamental electronic components, non-volatile memristors exhibit dynamic switching between high (HRS) and low resistance states (LRS) under electrical stimuli, which is essential for electronic memories, neuromorphic computing, and artificial intelligence.

High entropy Metal Organic Frameworks (MOFs) consist of metal ions connected by organic linkers, resulting in intricate structures with well-defined porosities, which leave spaces for ions, vacancies or guest molecules to immigration and provides an excellent environment for the electrochemical metallization (ECM) memristors. High-entropy materials, with entropy-stabilized structures and multivalent cation coordination, offer increased compositional complexity and tunable electrical properties. The combination of these characteristics makes high-entropy MOFs(HE-MOFs) a promising material platform for memristive devices.

We present novel HE-MOFs, integrated into resistive switching devices fabricated via microplotting and inkjet printing. The Ag/MOF/ITO memristors demonstrate reliable non-volatile ECM memristor, with an on/off ratio of 10^3.

Integrating MOFs into additive manufacturing techniques can revolutionize their applicability, opening doors to large-scale production of patterned MOF devices, also offering the benefits of low material waste, large range of patternable materials and compatible substrates. This work not only introduces new high-entropy MOFs but also establishes a practical platform for printable resistive memory devices.

CONSTRAINED SHAPE OPTIMISATION OF MILLING GEOMETRIES TO MINIMISE THERMAL STRESSES IN LAMELLA FOR CRYO-EM

Cornelis Mense

Cornelis Mense, Ulrich Schwarz, Roland Herzog

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Shape optimisation is an approach within the Finite Element Method, wherein geometry dependent derivatives are used to iteratively refine object shapes. It has traditionally been used in stress minimisation problems in engineering.

Here, we propose a scheme in which we calculate milling geometries that minimise stresses in lamella to decrease sample breakage in Cryo-EM. Shape derivatives are calculated using the automatic differentiation capabilities of FEniCS and are then applied under constraints that arise from experimental considerations. Constraints include a set amount of milled away material, along with Laplace-Beltrami smoothing that preserves the shape of outer surfaces.

The scheme is shown to significantly reduce thermal stresses by optimising the geometry, while maintaining imaging quality and milling time. Through these results, the scheme demonstrates shape optimisation as a general framework for solving geometry dependent optimisation problems under experimental constraints.

OBLIQUE PLANE MICROSCOPY WITH METASURFACES

Maryna L. Meretska

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A central challenge in modern neuroscience is to record the electrical activity of every neuron in a behaving animal with sufficient temporal resolution to resolve individual action potentials. Achieving this would require simultaneous measurements from approximately 10^5 neurons in small organisms such as larval zebrafish, and up to 8.6×10^{10} neurons in the human brain — each monitored with sub-millisecond precision.

Optical readout using calcium or voltage indicators currently provides one of the best compromises between spatial coverage, temporal resolution, and invasiveness. In transparent model organisms, whole-brain imaging with subcellular spatial resolution is already attainable using light-sheet or two-photon microscopy. However, extending these methods to capture fast neural dynamics in three dimensions at the required temporal bandwidth remains a considerable challenge.

Oblique plane light-sheet microscopy (OPM) has recently emerged as a promising strategy for high-speed volumetric imaging. By directing both excitation and detection through a single objective and requiring only one scanning mirror, OPM enables rapid imaging of large volumes. Nevertheless, the associated reimaging optics are complex and introduce substantial light losses, limiting overall performance. These losses can be significantly reduced by integrating custom-designed optical metasurfaces into OPM systems.

Optical metasurfaces — arrays of sub-wavelength nanostructures engineered to shape light with high precision — enable complete control over phase, amplitude, and polarisation. This technology has already yielded ultra-compact optical components, including polarimeters, imagers, and spectrometers, operating across broad wavelength ranges. Crucially, metasurfaces can be manufactured using standard CMOS-compatible processes, making them scalable and cost-effective.

Our work demonstrates that tailored metagratings can reduce optical losses in single-objective light-sheet microscopes. More broadly, metasurfaces provide a powerful and versatile platform for redesigning and optimising advanced imaging systems. We anticipate that this technology will play a key enabling role in the next generation of high-performance functional bioimaging tools.

SPATIALLY NONLOCAL METAMATERIALS FOR TAILORED ANOMALOUS DIFFUSION

Ke Wang

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In ordinary diffusion, the particle/heat/charge/mass flux at a given time and position is proportional to the local gradient of the chemical potential at the same position and time. However, in anomalous diffusion, the flux can also depend on the potential field at other positions and times, reflecting spatial and/or temporal nonlocality. Here we design two classes of spatially nonlocal metamaterials - thermal and fluid metamaterials - that enable the realization of anomalous diffusion behavior.

We designed 1D and 2D thermal metamaterials incorporating nonlocal connections of order N=2 and carried out time-dependent theoretical, numerical, and experimental studies, all of which revealed anomalous backward flow of heat induced by spatially nonlocal interactions. Furthermore, we designed 1D fluid-flow metamaterials with orders N=2,3,4, achieving backward flow of water under laminar regime, and this backward flow can be rationally designed by tailoring the nonlocal order N.

By utilizing nonlocal interactions, we design spatially thermal and fluid metamaterials that enable anomalous diffusion of heat and water flow. This anomalous diffusion can be rationally designed by customizing the order of nonlocal interactions, which unlock strategies for remote temperature sensing and improved fluid mixing.

INSIGHT INTO THE POLING BEHAVIOR OF MONOLITHIC ELECTROOPTIC MATERIALS

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The design of good electrooptic materials requires a high hyperpolarizability, good molecular alignment, and control over the absorption properties, as well as a high number-density. While hyperpolarizability is the most investigated property, here we focus on getting insight into the molecular alignments with respect to the external field axis. For this Replica Exchange Molecular Dynamics is employed (REMD).

MODULATING TWO-PHOTON ABSORPTION IN A PYRENE-BASED MOF SERIES: STRUCTURE-PROPERTY RELATIONSHIPS

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Metal-organic frameworks (MOFs) are emerging as promising materials for multiphoton absorption (MPA), a nonlinear optical phenomenon relevant for applications, such as bioimaging, phototherapy, and photonic devices.

However, the structural features that govern their exceptional MPA activity remain poorly understood. To address this, a family of pyrene-based MOFs (NU-1000, NU-901, SrTBAPy, and BaTBAPy), that vary in topology and secondary building units (SBUs), is systematically investigated.

Significant differences are observed in the two-photon absorption (2PA) cross-section σ(2), with BaTBAPy exhibiting the highest activity (8.2 × 104 GM). Quantum mechanical calculations reveal that intermolecular chromophore interactions and SBU-induced effects contribute strongly to enhanced σ(2) values, particularly in NU-901 and BaTBAPy.

The findings demonstrate that both framework topology and metal coordination environments are critical to modulating MPA behavior. These insights into the structure-property relationships of MOFs pave the way for rational design of next-generation nonlinear optical materials.

AN AUTOMATED WORKFLOW FOR PREDICTING FIRST HYPERPOLARIZABILITIES OF DONOR-ACCEPTOR CHROMOPHORES FOR NLO DEVICES

Jia Gao

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An accurate prediction of hyperpolarizability is essential for the development of advanced electro-optic materials. Several methods for calculating hyperpolarizability in different QM codes are reported in the literature.

It is known that the choice of method, e.g., the functional density functional theory (DFT), significantly impacts the reliability of these predictions. In this work, we showcase a streamlined simstack workflow for use with TURBOMOLE version 7.6, which is designed to compute and screen hyperpolarizability values efficiently, optimized for ease of use, and is intended for rapid identification and assessment of promising candidates for applications in nonlinear optics and related fields.

We also compare literature results across different functionals, which may help the end-user choose a method based on the systems they want to study.

A SERIES OF PRINTABLE GROUP 14 CHALCOGENIDE CLUSTERS WITH OPTICAL MULTIFUNCTIONALITY

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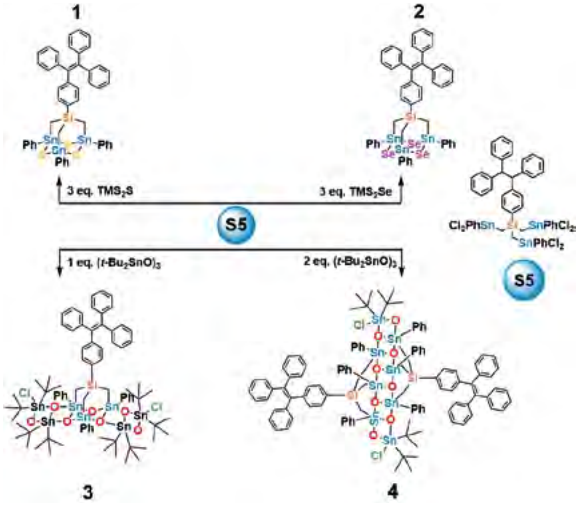
Tetrel chalcogenide clusters with organic substituents have long been studied for their structural, chemical, and physical properties.[1] A key class of these compounds has the formula $[(RT)_4E_6]$ (R = organic group; T = Si, Ge, Sn; E = S, Se, Te), where four organometallic units are connected by six chalcogenide ligands to form an adamantane-type core.[2-4]

Beyond purely organic or inorganic variants, hybrid organometallic adamantane-like clusters such as $[(RSi)\{CH_2Sn(E)Ph\}_3]$ (R = Phenyl, Naphthyl; E = S, Se,Te) have also been reported.[5,6] Inspired by these, we introduced the tetraphenylethene (TPE) ligand to synthesize a new series, $[(TPE\text{-}Si)\{CH_2Sn(E)Ph\}_3]$ (**1**: E = Se; **2**: E = S), which exhibit unique fluorescence absent in phenyl- or naphthyl-based analogs.

This prompted further exploration of oxygen incorporation via controlled oxygen source ratios, yielding compounds **3** $[(TPE\text{-}Si)\{CH_2Sn(O)Ph\}_3\{t\text{-}Bu_2SnO\}_4Cl_4]$ and **4** $[(TPE\text{-}Si)_2\{CH_2Sn(O)Ph\}_6\{t\text{-}Bu_2SnO\}_2Cl_2]$.



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ENHANCING TRIPLET EXCITONS LIFETIME THROUGH CONTROLLED INTERMOLECULAR INTERACTIONS

Martin Richter

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Singlet fission (SF) is a process in which a singlet exciton is converted into two triplet excitons, significantly enhancing charge generation in organic solar cells. It has been shown that the rate of SF and the lifetime of the generated triplet excitons strongly depend on the molecular arrangement.

In this work, a cofacial orientation of pentacene molecules is achieved by embedding organic linkers containing pentacene in a surface-anchored metal–organic framework. Transient absorption spectroscopy and a quantum mechanical analysis are used to analyze the exciton dynamics in a broad spectral range from near-ultraviolet to near-infrared. The observed spectra indicate that a singlet excited state generates a correlated triplet pair within a few picoseconds.

Subsequent dynamics show the formation of long-lived excitons (39µs) with triplet character. This exceeds by far the observed lifetime of triplet excitons generated in pentacene thin films and may enhance triplet exciton harvesting capabilities in photovoltaic cells.

DEVELOPMENT AND UNDERSTANDING OF ENANTIOSELECTIVE PASSERINI THREE COMPONENT REACTION

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Development and Understanding of Enantioselective Passerini Three Component Reaction.

APPLYING MACHINE LEARNING TO PREDICT PHOTOCHEMICAL ACTION PLOTS AND WAVELENGTH DEPENDENT QUANTUM YIELDS

Magdalena Unterreiner

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In 2017, the groups of Barner-Kowollik and Gescheidt have discovered an unexpected mismatch between molecular absorptivity and photochemical reactivity by developing the so-called photochemical action plot methodology. Action plots record the wavelength-dependent reactivity of photochemical reactions, which can often show a complex behavior and a red-shift of the reactivity compared to the absorption spectrum. A thorough understanding of the parameters that influence and control the outcome of photochemical reactions is necessary in order to conduct photochemical reactions in the most efficient fashion – including in the realm of light driven additive manufacturing.

The current project will explore the development and application of machine learning methods to predict and analyze physicochemical properties based on photochemical action plots.

Photochemical action plots provide high-dimensional datasets for data-driven analysis, but systematic evaluations have so far been limited. The project aims to address this gap by developing machine learning models capable of processing wavelength-resolved reactivity data obtained from experimental measurements or simulated sources. These models will be used to generate predictions of wavelength-dependent photochemical behavior.

Both existing and newly acquired photochemical datasets are intended to be used to evaluate model performance, robustness and transferability. Beyond establishing a suitable data basis, a key objective is to assess which types of predictions are feasible using machine learning in the context of photochemical action plots. In particular, the study will investigate whether it is possible to predict or rationalize the often-observed redshift between the maxima of absorption and reactivity. Identifying patterns or correlations within these datasets could provide new insights into photochemical mechanisms and open up previously unexplored predictive possibilities.

BEYOND NORRISH-TYPE REACTIVITY: A NOVEL PHOTOINITIATION MECHANISM FOR BIACETYL IN TWO-STEP TWO-COLOUR 3D MICROPRINTING

Vitalii Shekhovtsev

Vitalii Shekhovtsev, Jia Gao, Samira Gholami, Modan Liu, Joshua Futterer, Wolfgang Wenzel

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A detailed understanding of photoinitiation and chain-growth mechanisms remains a central challenge in polymer science, particularly for advanced 3D additive manufacturing technologies. The chemical identity of a photoinitiator not only determines the properties of the resulting polymer but also governs the underlying reaction pathways, thereby defining which printing strategies are accessible.

Here, we investigate the photoinitiation mechanism of acrylate photoresist polymerization triggered by biacetyl, a photoinitiator recently employed in two-color, two-step 3D printing. Our results show that biacetyl does not follow classical Norrish type I chemistry (homolytic C–C bond cleavage) nor a Norrish type II pathway (hydrogen abstraction) under typical printing conditions. Instead, biacetyl operates via a distinct photochemical mechanism that can support either a single-step, single-wavelength process or a two-step, dual-wavelength process, depending on the excitation wavelength.

These findings provide new mechanistic insight into wavelength-selective photopolymerization and establish a foundation for next-generation multicolor 3D printing strategies. More broadly, they demonstrate how tailored photoinitiator design can enable novel synthetic pathways and expand the functional capabilities of photopolymer-based additive manufacturing.

INVERSE DESIGN AND OPTIMIZATION OF A PHOTONIC COUPLER

Julius Paul Schmieta

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Photonic integrated circuits are seen as an alternative to traditional microelectronics based on semiconductors. Photonic integrated circuits offer a variety of benefits over traditional microelectronics, such as being more energy efficient and lower latencies. Efficiently coupling signals into photonic integrated circuits, for example between an on-chip waveguide and a fiber, is one of the main challenges which have to be addressed.

In this poster, I use inverse design methods to improve an existing top coupler design, which was designed using shape optimization, and adapt it to a different wavelength. That way, developing a coupler design for a different wavelength can be done by adapting an existing design, as opposed to developing a new design from the ground up.

The structures of interest are simulated using the adjoint method, which allows to obtain the gradient of an objective function relative to a set of input parameters by running two simulations, enabling gradient based optimization using an optimizer such as ADAM, which improves convergence of the optimization compared to non-gradient based methods.

The goal of the optimization is a bidirectional coupler that transforms any input so that it overlaps well with the mode of the second input. The geometry itself is generated using a 3D surface spline on a set of control points, which are the parameters used to optimize the design. That design is then converted into an array of permittivity values, similarly to density-based topology optimization. The final structures will then be fabricated using two-photon polymerization, allowing to validate the optimization results.

TOWARDS A FULLY DIFFERENTIABLE DIGITAL TWIN FOR SOLAR CELLS

Marie Louise Schubert

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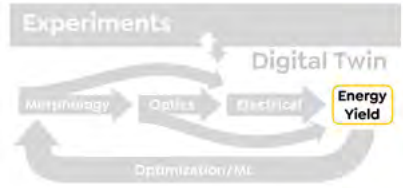
Emerging photovoltaic (PV) technologies enable lightweight, flexible, and multi-benefit energy solutions that surpass the traditional silicon-based modules. Advances in materials and device engineering, supported by numerical simulations, have accelerated performance optimization and reduced development costs [1]. While simulation tools play a crucial role in advancing emerging PV research, many simulation frameworks focus on individual sub-components of solar cells, limiting their ability to optimize the total energy yield (EY) of complex PV architectures.

To address this challenge, we present a holistic, differentiable digital twin that calculates the EY from key input parameters, including the materials used in the device, its general geometry, and specific processing conditions [2]. The digital twin enables the computational assessment of all parameters characterizing a solar cell at its various stages, once the details of the device are set.

To exemplify the framework, we choose to consider an organic solar cell with the photoactive OPV material PM6:Y6. Our workflow integrates morphological modeling, optical simulations, electrical calculations, and device modeling into one unified framework to compute the EY. Surrogate machine-learning models are introduced for highly complex simulations. The differentiable design of the digital twin enables end-to-end optimization and the systematic study of EY dependencies, and the framework identifies optimal design parameters to maximize the EY using a gradient-based approach. The digital twin is initially applied to an organic PV module evaluated across different climates.



While demonstrated here for organic solar cells, the workflow is generic and can be adapted to other PV technologies. The proposed digital twin marks a significant step towards tailored PV systems for various applications and EY driven optimization.

Figure 1: Schematic of the digital twin

[1] L. Lüer et al. "A digital twin to overcome long-time challenges in photovoltaics". In: Joule 8.2 (2024). DOI: 10.1016/j.joule.2023.12.010.
[2] M.L. Schubert et al. "Towards a fully differentiable digital twin for solar cells". *In preparation*

FROM MOLECULES TO METASURFACES: FAST MULTISCALE MODELING OF THERMAL EMISSION

Martin Gabbert

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Thermal emission, the electromagnetic radiation emitted by a body due to its temperature, is ubiquitous. Its control underpins important applications such as thermophotovoltaic energy harvesting, and radiative cooling. Photonic systems for the control of thermal radiation can benefit from platforms made available by modern micro- and nanofabrication, including micro-structured bulk materials, molecular films, and atomic monolayers. Exploiting such a complex design space requires accurate and computationally efficient tools, which enable computer-aided design and the reliable interpretation of experiments. Thermal-emission calculations are particularly demanding: Planck's law results in large bandwidths, and the radiation from micro-structured materials must also be resolved with respect to direction and polarization. Therefore, the field of thermal photonics requires accurate and efficient tools able to handle the aforementioned complexity.

I will present how we extended a multiscale scattering framework [1,2] to compute thermal emission spectra from molecules, particles, clusters and arrays thereof, and planar cavities. Examples include a single molecule [3] and a metasurface of maximally chiral particles [4], the latter of which exhibits multiple directionally broad emission bands with strongly polarized radiation. For metasurfaces, our method is one to two orders of magnitude faster than state-of-the-art methods, with further improvements possible.

We will advance towards the inverse design of metasurfaces for thermal applications using automatic differentiation and gradient-based optimization. We will also study thermal radiation in highly chiral cavities [5], and explore systems ranging from two-dimensional materials to relativistically moving emitters.

[1] D. Beutel, I. Fernandez-Corbaton, and C. Rockstuhl, Comput. Phys. Commun., 297, 109076, 2024.
[2] B. Zerulla, et. al., Adv. Mater., 34, 2200349, 2022.
[3] J. D. Mazo-Vasquez, et. al., Phys. Rev. B 112, 054307, 2025.
[4] M. Gabbert, et al., Under review in PRB, arXiv:2508.11590, 2025.
[5] L. Rebholz, C. Rockstuhl, and I. Fernandez-Corbaton, Under review in PRL, arXiv:2507.10481, 2025.

T-MATRIX-BASED MULTIPLE-SCATTERING MODELING OF ACOUSTIC METAMATERIALS AND METASURFACES

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Spatially ordered arrays of acoustic scatterers, such as metamaterials and metasurfaces, offer numerous possibilities for manipulating sound and ultrasound waves at the subwavelength scale, beyond what is achievable with natural materials.

Simulating the acoustic response of metamaterials constitutes a multiple-scattering problem, which can be efficiently addressed using the T-matrix method. In this contribution, we report on textit{acoustotreams}, a computational framework that enables fast and accurate scattering calculations in Python for one-, two-, and three-dimensional lattices of scatterers with arbitrary geometries.

We further demonstrate two representative applications of the program: the description of bound states in the continuum and the effective properties of acoustic metamaterials.

The results are validated through comparison with COMSOL Multiphysics simulations and experimental data.

APPLICATIONS OF A MULTISCALE FRAMEWORK FOR NONLINEAR OPTICAL SIMULATIONS IN PERIODIC STRUCTURES

Mariia Poleva

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We present a framework to simulate the nonlinear optical response of periodic structures using the hyper-T-matrix formalism [1], which connects incident and scattered field coefficients at the unit-cell level. This approach enables efficient computation of the nonlinear response of the entire structure. The workflow is implemented in the in-house, open-source software treams [2].

A key application is the first-principles study of molecular materials: the unit cell is analyzed using quantum-chemical simulations to obtain its hyper-T-matrix, which is then combined with Maxwell simulations to predict the nonlinear scattering of the periodic material. This multi-scale approach allows the simulation of the optical response of large molecular systems that exceed the limits of purely quantum-mechanical descriptions.

We illustrate the approach with two examples. The first involves 7-layer gold–cysteine nanoparticles in solution, where including the electrostatic influence of surrounding layers via layer-specific partial-charge embedding enables simulations to accurately reproduce experimental trends [3]. The second example considers second-harmonic generation (SH) in thin-film stacks of three distinct metal-organic frameworks, highlighting how the stacking arrangement and cavity resonances influence the overall SH intensity.

Our method also applies to metasurfaces with subwavelength meta-atoms, whose hyper-T-matrices are obtained via full-wave simulations.

[1] B. Zerulla et al.: Adv. Mater. 36, 2311405 (2024).
[2] D. Beutel et al.: Comput. Phys. Commun. 297, 109076 (2024).
[3] M. Poleva et al.: J. Phys. Chem. C 129, 17119 (2025).

INVERSE DESIGN OF 3D NANOPHOTONIC DEVICES

Oliver Kuster

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Recent developments in 3D nanoprinting allow us to print devices that can manipulate light at subwavelength scale. The design of such compact and highly efficient nanophotonic devices also requires highly efficient optimization methods to go along with them. In recent years, inverse design has been incredibly successful in the design of 2D nanophotonic devices. By leveraging a gradient-based optimization approach, inverse design is able to accommodate millions of degrees of freedom in the optimization process. Transitioning to 3D, a new dimension becomes accessible in the design space, allowing for even more efficient devices compared to traditional 2D designs.

However, this transition to using 3D nanoprinting for the design process comes with additional challenges. This work presents an inverse design pipeline to create a digital blueprint for 3D nanoprinting and addresses these additional challenges in the optimization procedure itself. A model of the physical printing process is used to replace the traditional filtering process in inverse design. By modelling the point spread function of the laser to represent the energy deposition into the polymer, we are able to model the printed design and optimize its optical response. This means that every design found by the optimizer is not only printable but also optimized for the printing technology itself.

Furthermore, we use a virtual heat method to ensure the structural integrity of our design and use robust topology optimization to increase the tolerance of the design with respect to fabrication variations. Combined, we obtain an inverse design pipeline that can provide a wide range of 3D printable nanophotonic devices on demand, without the need for postprocessing.

Thank You

DEAR COLLEAGUES AND FRIENDS,

We want to take this opportunity to thank everyone involved in this conference: the invited speakers as well as the participants with or without oral and poster presentations.

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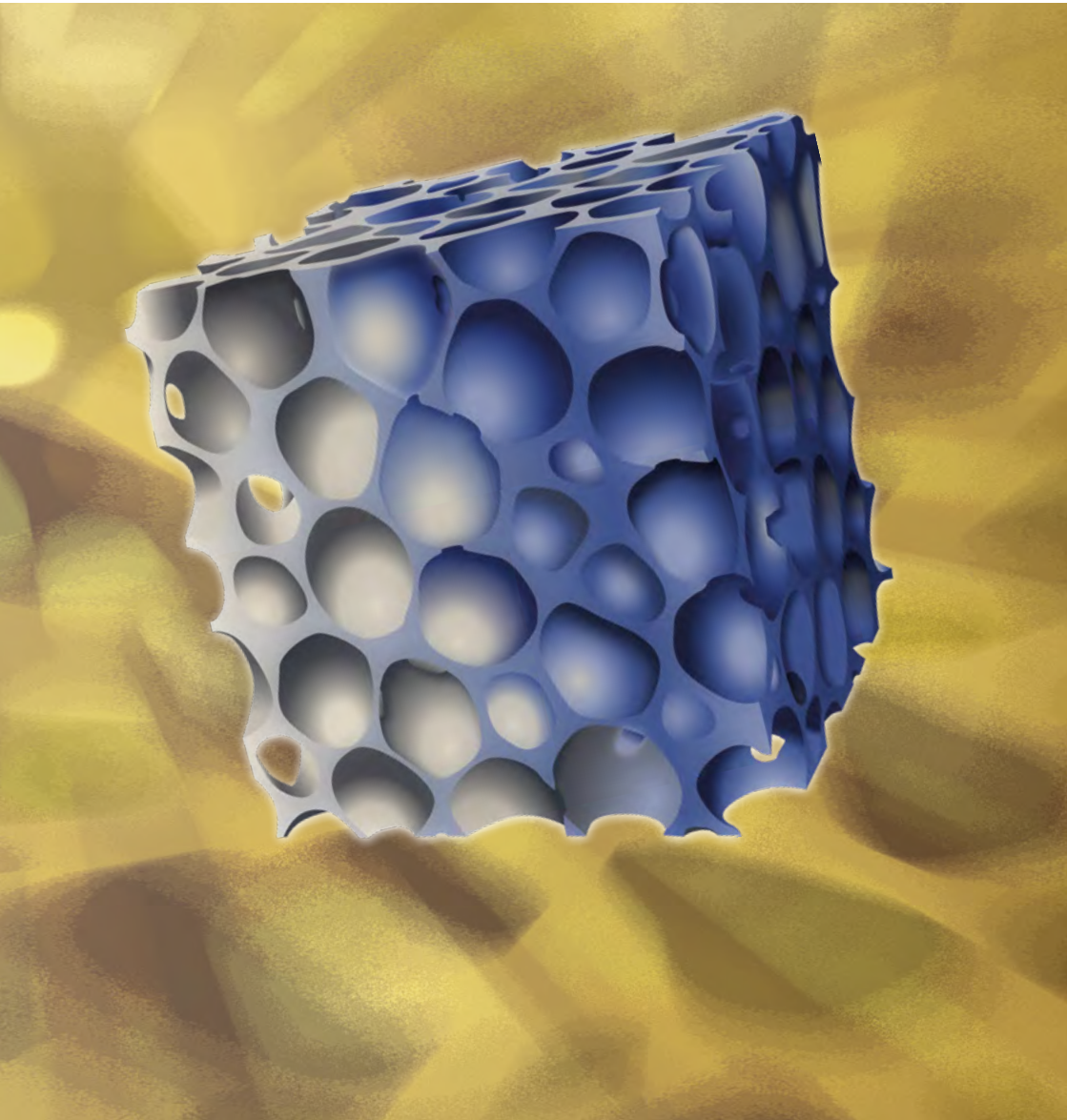

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