20th ANNIVERSARY
NSDays 2024

ABSTRACT BOOK

NSC
FINLAND

UNIVERSITY OF JYVÄSKYLÄ

Tuesday 8.10.2024

AGORA LOBBY

09:00 Music, coffee and registration

MARTTI AHTISAARI HALL

09:30 Opening words, Rector Jari Ojala

Session I

09:45 **Jukka Pekola,** Aalto University
Quantum thermodynamics in superconducting circuits

10:45 **Harry Andersson,** University of Oxford
Molecular wires and nanorings

11:45 Lunch break and setting up posters

MARTTI AHTISAARI HALL

Session II

13:00 **Johann Peter Reithmaier,** University of Kassel
Nanostructured semiconductors for photonic and optoelectronic applications

14:00 **Jens Bosse,** Hannover Medical School
From in-silico to in cellulo - Illuminating viral morphogenesis

AGORA LOBBY

15:00-17:00 Poster session and wine

AALTO HALL

17:30 Arriving to the anniversary dinner
17:45 Speech by former Rector Matti Manninen
18:00 Panel discussion
19:00- Anniversary dinner and evening programme
Äänes and Nanöband

Wednesday 9.10.2024

MARTTI AHTISAARI HALL

Session III

HONORARY SPEAKER

09:00 **Morten Meldal,** University of Copenhagen
Molecular click adventures – a leap from the shoulders of giants

10:00 Coffee

Session IV

10:30 **Sandrine Bourdoulous,** The National Centre for Scientific Research
New strategies to fight bacterial sepsis - the example of Neisseria meningitidis

11:30 **Sponsor session**
CEO Kim Törnqvist, Cheos Oy
Imaging techniques for a wide spectral range
Innovation Manager Nicholas Hendricks, Heidelberg Instruments
The next generation NanoFrazor - a modular approach to micro and nanofabrication
Mikael Friberg, Merck
Introduction to Merck Life Science

11:45 Lunch break

MARTTI AHTISAARI HALL

Session V

13:00 **Molly Stevens (online),** University of Oxford
Designing new nanomaterials for tissue regeneration and therapeutics

14:00 **Päivi Törmä,** Aalto University
Quantum geometry in superconducting and photonic systems

15:00 Closing ceremony

Plenary speakers

1. **Jukka Pekola**

   Quantum thermodynamics in superconducting circuits

2. **Harry Andersson**

   Molecular wires and nanorings

3. **Johann Peter Reithmaier**

   Nanostructured semiconductors for photonic and optoelectronic applications

4. **Jens Bosse**

   From in-silico to in cellulo - illuminating viral morphogenesis

5. **HONORARY SPEAKER: Morten Meldal**

   Molecular click adventures – a leap from the shoulders of giants

6. **Sandrine Bourdoulous**

   New strategies to fight bacterial sepsis - the example of Neisseria meningitidis

7. **Molly Stevens (online)**

   Designing new nanomaterials for tissue regeneration and therapeutics

8. **Päivi Törmä**

   Quantum geometry in superconducting and photonic systems

Plenary I

Quantum thermodynamics in superconducting circuits

Jukka Pekola[1*]

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Recent fast progress in developing superconducting circuits mainly for quantum information processing purposes enables researchers to employ them also in various other types of investigations and applications. My group's speciality is to couple these circuit QED structures to on-chip heat baths formed of normal metals with controllable temperatures and sensitive thermometry. I will review the work for which we laid the basis already in 1990's at the University of Jyväskylä, and then I move to our recent and ongoing work on superconducting qubits in studies of quantum heat transport, heat valves and diodes, heat engines, thermometers etc. The combination with heat baths made of metallic or graphene absorbers, allows for ultrasensitive bolometry and calorimetry of quantum systems, e.g., with promise of wide-band single quantum detection in the microwave regime. I will also highlight the potential of superconducting circuits as highly controlled open quantum systems, and on the other hand as virtually isolated quantum systems for fundamental studies of thermalization.

Plenary II

Molecular wires and nanorings

Harry Andersson[1*]

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Molecular wires are the most fundamental single-molecule electronic device and the molecular components of organic semiconductors. This lecture will present recent results on the investigation of molecular wires derived from porphyrins. Porphyrins are the 'colours of life' – they make blood red and grass green; they also survive for millions of years in minerals. They can be used to construct molecular wires and nanorings that mediate efficient charge transport over distances of several nanometers. Their small reorganization energies lead to low barriers for charge transport and they are remarkably amenable to template-directed synthesis, providing access to nanorings and other architectures. Recent work on π-conjugated porphyrin arrays will be presented.

Plenary III

Nanostructured semiconductors for photonic and optoelectronic applications

Johann Peter Reithmaier,[1*] Mohamed Benyoucef[1] and Cyril Popov[1]

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An overview is given about the group activities on the development of nanostructured materials, which includes III-V compound semiconductors as well as diamond. Several major areas of applications are addressed, such as quantum dot gain materials for diode lasers, single photon emitting structures for quantum key distribution and photonic structures in diamond to enhance light matter interaction with embedded color centers.

Record values in temperature stability, modulation speed and ultra-narrow linewidth in InP-QD lasers were obtained in the recent years, which exhibit superior performance and indicate the potential to outperform in future state of the art QW lasers.

Due to possible geometric asymmetries in QD structures, the entanglement of polarization states is not possible, which results in a finite fine structure splitting (FSS). In more recent results based on a specific growth technique, the symmetry of semiconductor quantum dots can be significantly improved on InP-based QDs, which results in very low FSS values in the order of the lifetime limited linewidth. These single photon emitters are key devices for long range fiber-based quantum key distribution systems operating at 1.5 µm.

A very promising material system for quantum technology applications, such as quantum memory or quantum processing, are diamond structures with embedded color centers, e.g., NV or SiV centers. However, the light interaction with a single atom-like dipole is rather low, and the light-matter interaction must be enhanced by photonic nanostructures. However, the fabrication of nanopillar or nanocavities in diamond is much more challenging than in conventional compound semiconductors. In the recent years, many nanoscale photonic structures were developed, which includes ultra-smooth surfaces, nanopillars and photonic crystal based structures in diamond.

Plenary IV

From in-silico to in cellulo - illuminating viral morphogenesis

Jens Bosse[1,2*]

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Herpesviruses encode for hundreds of proteins, many of which are needed to assemble to form infectious particles that can transmit the viral genome and establish a consecutive, productive infection cycle. It is mostly unknown how all these factors are assembled and brought together in an infected, living cell at the single-particle level. Using the recent developments in AI-driven structural predictions, we have generated a comprehensive and stringently scored structural prediction database of all human herpesviruses proteins as well as their complexes. These data are freely accessible at www.bosse-lab.org/herpesfolds. By integrating these structural predictions with live-cell microscopy, CLEM and Cryo-EM, we are unraveling how viral factors interact over space and time in infected cells. I will illustrate this approach along our recent findings of a previously unkown family of viral proteins that mediate viral replication.

HONORARY SPEAKER / Plenary V

Molecular click adventures – a leap from the shoulders of giants

Morten Meldal[1*]

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The concept of click chemistry matured simultaneously in different laboratories around the world in the 1990's. There was an urgent need for quantitative chemical reactions to cope with the pressure from combinatorial science to synthesize, screen and identify millions of compounds. We serendipitously discovered the CuAAC click reaction in 2001. The mechanism of the reaction will be discussed, and its applications will be presented, as well as existential aspects of our fundamental understanding of chemistry and the importance of serendipity.

Plenary VI

Mechanisms regulating the traffic of leukocytes and cancer cells in the body

Sandrine Bourdoulous[1,2*]

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Our team has a long-standing interest in vascular cell biology in the context of infection and inflammation, in particular at the central nervous system level, where the blood-brain barrier tightly controls neuronal environment. Endothelial cells are major targets of sepsis-induced events. A wide range of invasive pathogens directly target endothelial cells and affect most aspects of endothelial cell biology, leading to edema, occlusive clotting, excessive inflammation and organ failure. Among them, Neisseria meningitidis (meningococcus) is still a leading cause of two rare but devastating invasive diseases: meningitis and severe sepsis (purpura fulminans). We have developed interdisciplinary approaches to elucidate the intricated network of interactions and molecular strategies elicited by this bacterial pathogen to colonize human vasculature, promote vascular dysfunction and get access to the brain. Our original research led to the identification of innovative therapeutic strategies to combat bacteria-induced severe endothelial dysfunction. We identified compounds against Type IV pili, a major virulence factor found in numerous bacterial pathogens, which contributes to meningococcal pathogenesis by promoting vascular colonization and subsequent vascular alteration. More recently, we identified a potent vascular stabilization factor conferring protection against severe bacterial sepsis.

Plenary VII (online)

Designing new nanomaterials for tissue regeneration and therapeutics

Molly Stevens[1*]

[2]*Department of Physiology, Anatomy, & Genetics, Department of Engineering Science, and Kavli Institute for Nanoscience Discovery, University of Oxford, Oxford, OX1 3QU, UK*

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This talk will provide an overview of our recent developments in bioinspired materials for applications in advanced therapeutics and biosensing with focus on establishing translational pipelines to bring our innovations to the clinic [1]. Our group has developed fabrication methods to engineer complex 3D architectures that mimic anisotropic and multiscale tissue structures and generate spatially arranged bioinstructive biochemical cues [2]. I will discuss recent advances in our tunable nanoneedle arrays for multiplexed intracellular biosensing at sub-cellular resolution and modulation of biological processes [3]. We are developing creative solutions for targeted and controlled delivery using microrobots with unique bioinspired characteristics that respond to external stimuli to release a payload [4]. Our therapeutic delivery portfolio includes high molecular weight polymer carriers for enhanced delivery of saRNA therapeutics and photo-responsive nanoreactors inspired in the circadian rhythms [5]. We are exploiting the sensing capabilities of functionalised nanoparticles to engineer nanoprobes for in vivo disease diagnostics that produce a colorimetric response ideal for naked eye read-out and for CRISPR-based preamplification free detection of ncRNAs (CrisprZyme) which we have validated with cardiovascular disease patient samples [6]. I will present advances in Raman spectroscopy for high-throughput label-free characterization of single nanoparticles (SPARTA™) that allow us to integrally analyse a broad range bio-nanomaterials without any modification enabling exciting biosensing applications using extracellular vesicles as disease biomarkers, a growing area of interest in cardiovascular medicine [7]. Finally, I will explore how these versatile technologies can be applied to transformative biomedical innovations and will discuss our efforts in establishing effective translational pipelines to drive our innovations to clinical application while actively engaging in efforts towards the democratisation of healthcare [8].

References

[1] J. P. K. Armstrong *et al. Sci. Transl. Med.* 12, 572, eaaz2253, (2020).
[2] T. von Erlach *et al., Nat. Mater.* **17**, 237-242, (2018).
[3] C. Chiappini *et al. Nat. Mater.* **14**, 532, (2015).
[4] X. Song *et al. Adv. Mater.* **34**, 43, 2204791, (2022); R. Sun et al. *Adv. Mater.* **35**, 13, 2207791, (2022).
[5] A. Blakney *et al. ACS Nano.* **14**, 5, 5711-5727, (2020); O. Rifaie-Graham *et al., Nat. Chem.* 15, 110–118, (2023).
[6] C. N. Loynachan *et al. Nat. Nanotechnol.* **14**, 883-890, (2019); M. Broto *et al. Nat. Nanotechnol.* **10**, 1038, (2022).
[7] J. Penders *et al. Nat. Commun.* **9**: 4256, (2018); J. Penders *et al. ACS Nano*. 15, 11, 18192–18205, (2021); H. Barriga *et al. Adv. Mater.* **34**, 26, 2200839, (2021).
[8] Speidel, A.T., Grigsby, C.L. and Stevens, M.M. *Nat. Mater.* **21**, 989–992 (2022).

Plenary VIII

Quantum geometry in superconducting and photonic systems

Päivi Törmä[1*]

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We discuss the role of quantum geometry in superconductivity, where it enables supercurrents in flat bands. Recent results on non-equilibrium transport in flat band superconductors and temperature dependence of the quantum geometric superfluid stiffness are presented, and their relation to recent experiments in twisted bilayer graphene. We then switch to topological photonics and discuss quantum metric measurements as well as high topological charge lasing in plasmonic quasicrystals.

POSTER PRESENTATIONS

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Contents

Poster 1

DAM! – Novel AFM-based deposition analysis method in selective protein functionalization of graphene devices for neurotransmitter detection

Aku Lampinen[1], Johanna Schirmer[1], Aleksei Emelianov[1], Andreas Johansson[1,2], Mika Pettersson[1]
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Functionalization of graphene is essential for it to be used as a molecule-specific biomolecule detecting platform. [1–3] Therefore, utilizing different methods of functionalization has attracted significant attention. [4] Atomic force microscopy (AFM) is a useful technique for determination of coverage and selectivity of functionalized surfaces for 2D materials. However, the analysis of functionalization results is not straightforward, and the results often depend on user-specified parameters, which hinders systematic design of functionalization strategies. To address this problem, we report on a novel histogram-based semi-automatic atomic force microscopy (AFM) deposition analysis method (DAM) that can reasonably accurately determine the thickness, coverage, and the amount of functionalized material on the surface of a 2D material. The DAM demonstrates superiority over commonly used methods, such as cross-section-based analysis, which suffer from significant user error and the selection of arbitrary values, leading to poor systematics.

DAM was applied for the analysis of non-covalent protein functionalization of graphene utilizing laser-induced two-photon oxidation (2PO) as a way to control the selectivity of functionalization and level of deposition. [5] The challenge was to detect reliably differences in protein binding on pristine and photo-oxidized graphene as a function of irradiation dose. The results show that DAM is able to reveal systematic differences in deposition thickness and coverage. The results are applied for development of graphene field effect transistor (GFET) devices functionalized with calmodulin and acetylcholine receptor fragment [5] for neurotransmitter biosensors.

References

[1] S. Kumar, Y. Pramudya, K. Müller, A. Chandresh, S. Dehm, S. Heidrich, A. Fediai, D. Parmar, D. Perera, M. Rommel, L. Heinke, W. Wenzel, C. Wöll, and R. Krupke, *Advanced Materials* **33**, 2103316 (2021).

[2] X. Zhang, Q. Jing, S. Ao, G. F. Schneider, D. Kireev, Z. Zhang, and W. Fu, *Small* **16**, 1902820 (2020).

[3] L. von Lüders, R. Tilmann, K. Lee, C. Bartlam, T. Stimpel-Lindner, T. K. Nevanen, K. Iljin, K. C. Knirsch, A. Hirsch, and G. S. Duesberg, *Angewandte Chemie* **135**, e202219024 (2023).

[4] P. Suvarnaphaet and S. Pechprasarn, *Sensors* **17**, 2161 (2017).

[5] A. Lampinen, J. Schirmer, A. Emelianov, A. Johansson, and M. Pettersson, *RSC Applied Interfaces*, Advance article (2024).

Tube-shaped assemblies of DNA-origami-lattices in solution

J. M. Parikka[1], H. Järvinen[1], K. Sokołowska[1], V. Ruokolainen[2], N. Markešević[1], A. K. Natarajan[3], M. Vihinen-Ranta[2], A. Kuzyk[3], K. Tapio[1], J. J. Toppari[1]

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Hierarchical self-assembly of nanostructures with addressable complexity has been a promising route for realizing novel functional materials [1]. Traditionally, the fabrication of such structures on a large scale has been achievable using top-down methods but with the cost of complexity of the fabrication equipment versus resolution and limitation mainly to 2D structures. More recently bottom-up methods using molecules like DNA have gained attention due to the advantages of low fabrication costs, high resolution, and simplicity in an extension of the methods to the third dimension [2]. One of the more promising bottom-up techniques is DNA origami due to the robust self-assembly of arbitrarily shaped nanostructures with feature sizes down to a few nanometers.

Here, we show that under specific ionic conditions of the buffer, the employed plus-shaped, blunt-ended Seeman tile (ST) [3] origami forms elongated, ordered 2D lattices, which are further rolled into 3D tubes in solution [4]. Imaging structures on a surface by atomic force microscopy reveals ribbon-like structures, with single or double layers of the origami lattice. Further studies of the double-layered structures in a liquid state by confocal microscopy and cryo-TEM revealed elongated tube structures with a relatively uniform width but with a varying length. Through meticulous study, we concluded that the assembly process of these 3D DNA origami tubes is heavily dependent on the concentration of both mono- and divalent cations. In particular, nickel seems to act as a trigger for the formation of the tubular assemblies in liquid, as depicted in figure 1.

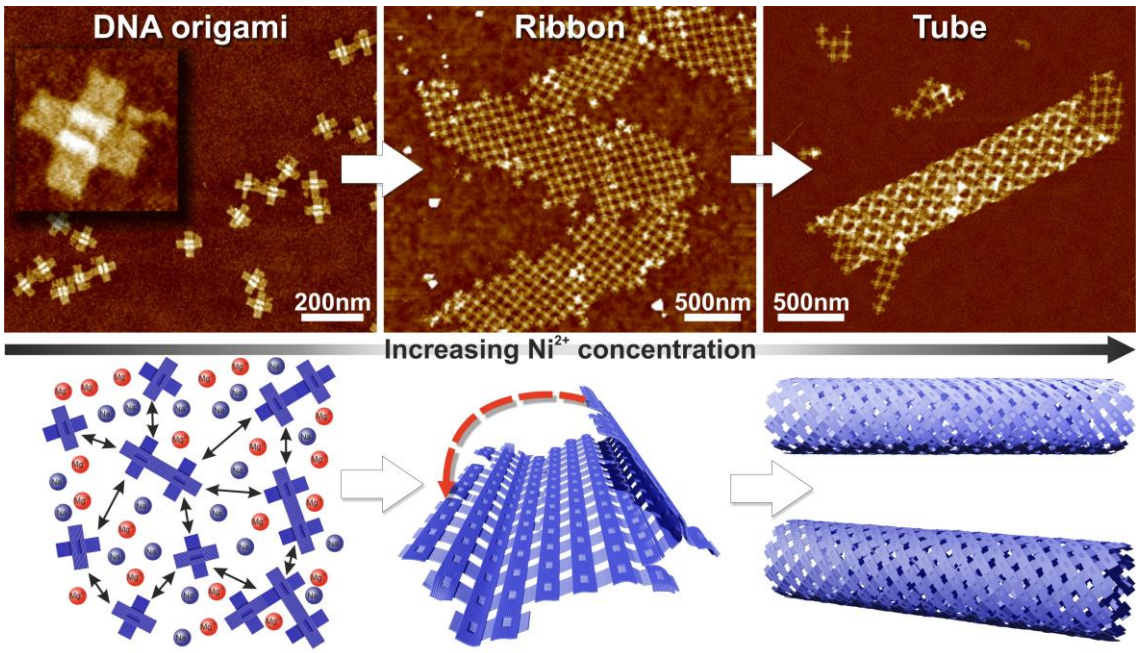

Figure 1: ST assembly formation with increasing nickel concentration.

References

[1] F. Hong, F. Zhang, Y. Liu, *et al.*, *Chemical reviews* **117**, 12584–12640 (2017).

[2] T. Zhang, *et al.*, *Adv. Mat.* **30**, 1800273 (2018) ; S.H. Park, *et al.*, *Nanophotonics* **12**, 2611–2621 (2023).

[3] W. Liu, *et al.*, *Angew. Chem.* **50**, 264–267 (2011) ; A. Rafat, *et al.*, *Angew. Chem.* **53**, 7665–7668 (2014).

[4] J.M. Parikka, H. Järvinen, K. Sokołowska, *et al.*, *Nanoscale* **15**, 7772–7780 (2023).

Simulating Quantum Effects in Electronic Strong Coupling

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We investigate and compare simulations of the collective coupling of an ensemble of molecules to a cavity field using semi-classical hybrid quantum mechanics/molecular mechanics (QM/MM) and multi-configuration time-dependent Hartree (MCTDH) approaches. We aim to validate the semi-classical molecular dynamics (MD) and assess the role of quantum effects in the relaxation processes. Initially, we considered a diatomic CO molecule and optimized its equilibrium geometry at the electronic ground state using the CCSD/aug-cc-pVDZ level of theory with the G09 program. The first six singlet low-lying electronic states were calculated using the CASSCF (14,10) ab initio quantum chemistry method along the CO internuclear distance. We then constructed the Tavis-Cummings model Hamiltonian by considering the ground and first excited electronic states of the CO molecule within the rotating wave approximation. Simulations were performed using both QM/MM and MCTDH approaches. Our simulations show that the results are qualitatively in agreement when a single CO molecule is coupled to the cavity mode. The project involving multiple molecules is still in progress.

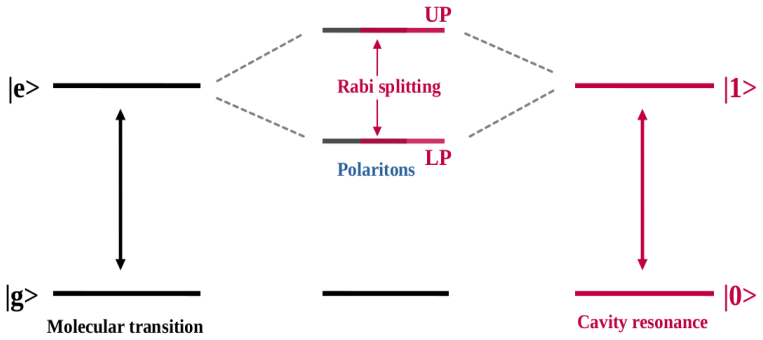

Figure 1: Schematic picture of molecule-cavity interaction.

References

[1] M. Tavis and F. W. Cummings, Phys. Rev. **188**, 692 (1969).

[2] O. Vendrell, Phys. Rev. Let. **121**, 253001 (2018).

[3] R. H. Tichauer, J. Feist, and G. Gorenhof, J. Chem. Phys., **154**, 104112 (2021).

[4] I. S. Ulusoy, J. A. Gomez, and O. Vendrell, J. Phys. Chem. A **123**, 8832 (2019).

Large-Scale Formation of DNA Origami Lattices on Silicon

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In recent years, hierarchical nanostructures have found applications in fields like diagnostics, medicine, nano-optics, and nanoelectronics, especially in challenging applications like the creation of metasurfaces with unique optical properties [1]. One of the promising materials to fabricate such nanostructures has been DNA due to its robust self-assembly properties and plethora of different functionalization schemes [2].

Here, we demonstrate the assembly of a two-dimensional fishnet-type lattice on a silicon substrate using cross-shaped DNA origami as the building block, *i.e.*, tile [3]. The effects of different environmental and structural factors are investigated under liquid atomic force microscopy (AFM) to optimize the lattice assembly. Effects of incubation time and sodium concentration at 35 °C temperature is shown in figure 1. Furthermore, the arm-to-arm binding affinity of the tiles is analyzed, revealing preferential orientations. From the liquid AFM results, we developed a methodology to produce closely spaced DNA origami lattices on silicon substrate. Similar lattices have been formed on the common mica substrate [4], but the importance of silicon is that it allows further nanofabrication process steps, such as metallization. This formed polycrystalline lattice has high surface coverage and is extendable to the wafer scale with an average domain size of about a micrometer. Further studies are ongoing to increase the domain size toward a single-crystalline large-scale lattices.

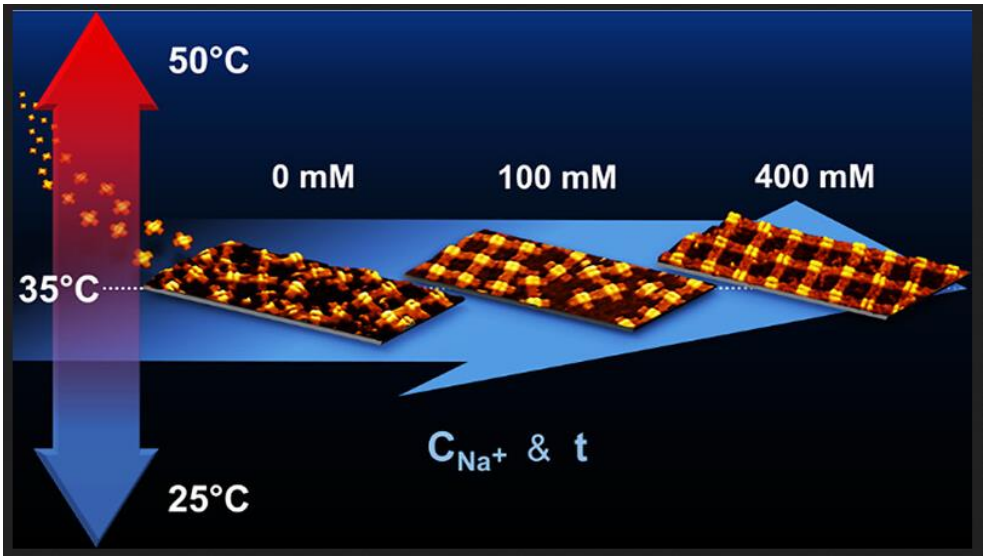

Figure 1: ST lattice formation with increasing time and sodium concentration.

References

[1] L. Lermusiaux, L. Roach, A. Baron, M. Tréguer-Delapierre, *Nano Ex.* **3**, 021003 (2022).

[2] F. Hong, F. Zhang, Y. Liu, et al., *Chemical reviews* **117**, 12584–12640 (2017).

[3] K. Tapio, C. Kielar, J.M. Parikka, A. Keller, H. Järvinen, K. Fahmy and J.J. Toppari, *Chem. Mater.* **35**, 1961-1971 (2023).

[4] J.M. Parikka, K. Sokołowska, N. Markešević, and J.J. Toppari, *Molecules* **26**, 1502 (2021).

Poster 5

Development of a bioinformatics pipeline for the study of CRISPR evolution in the human gut microbiome.

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Keywords: CRISPR, microbiome, bioinformatics

CRISPR-Cas systems are part of bacterial and archaeal defence systems against invading genetic elements. A key feature of CRISPR-Cas systems is that the CRISPR array component can serve as a temporal record of previous infections due to the integration of spacer sequences into the CRISPR array upon infection. The CRISPR-Cas systems primarily target bacteriophages, although they also target other mobile elements such as mobile plasmids.

The role of the dynamics between the gut viriome and microbiome in human health is an area of increasing research interest. Multiple studies have indicated that the dynamics between the gut microbiome and phageome are affected by external selection pressures, such as antibiotic therapy.

Despite this, little research has been done to determine how antibiotics can shift the bacterial CRISPR-phage-plasmid dynamics and CRISPR evolution in the gut community. The aim of this project is to develop a pipeline that can elucidate how these dynamics evolve over time using metagenomic data, and to apply this pipeline to metagenomic data of human gut microbial samples following antimicrobial therapy.

Photocleavable BODIPY-derivatives for light-induced patterning of graphene surface

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Photocleavable protecting groups (PPGs) are molecules that go through selective light-induced bond breaking. In other words, PPGs allow the *in situ* release of bioactive molecules with light, which is beneficial for biomaterial applications and chemical surface modification [1]. Boron-dipyrromethene (BODIPY) compounds are a class of PPGs that can be removed with visible light tuned to occur in green-to-red-light regions [2,3]. BODIPY-based PPGs are especially useful for biological and medical applications because visible light is less harmful than UV light required to deprotect many other PPGs [1].

We have synthesized three BODIPY-bearing photocleavable compounds **1**-**3** differing from the size of the aromatic end group (Figure 1). Chemical structures were designed for non-covalent attachment on graphene surface through π-π stacking interaction (Figure 1b). The compounds' photochemical properties were studied by UV-vis and fluorescence spectroscopies, and their photocleavage in solution in ambient and inert atmosphere with NMR and HR-MS spectroscopies. The compounds have similar photophysical properties and photocleavage mechanisms. In addition, we have shown that the compounds can be deposited on graphene and selectively cleaved with green light while creating different patterns on graphene [4]. The patterns were visible on AFM images and with Raman mapping. This is a step toward our ultimate goal of guiding neuron growth on graphene surfaces with light utilizing these compounds.

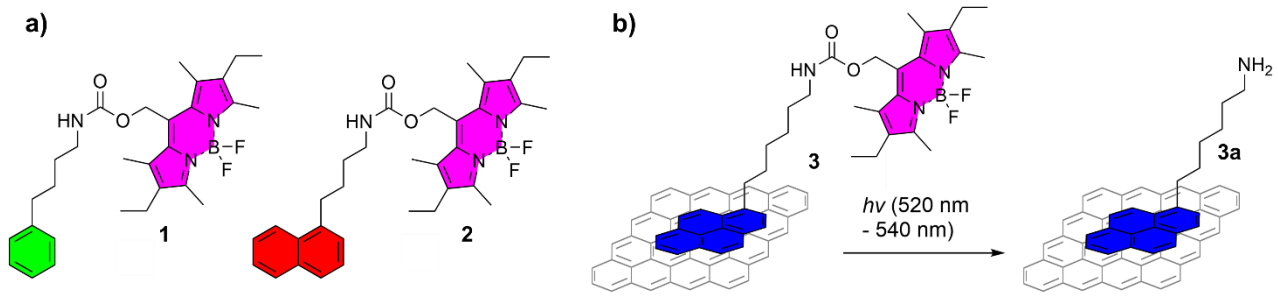

Figure 1. a) Chemical structures of synthesized compounds **1** and **2**. b) Schematic presentation of π-π interaction between graphene and BODIPY-protected amine (**3**) and the outcome after irradiation with green light.

References

[1] R. Weinstain, T. Slanina, D. Kand, and P. Klán, *Chem. Rev.* **120**, 13135–13272 (2020)
[2] D. Kand, P. Liu, M. X. Navarro, L. J. Fischer, L. Rousso-Noori, D. Friedmann-Morvinski, A. H. Winter, E. W. Miller, and R. Weinstain, *J. Am. Chem. Soc.* **142**, 4970–4974 (2020)
[3] K. Sitkowska, M. F. Hoes, M. M. Lerch, L. N. Lameijer, P. van der Meer, W. Szymański, and B. L. Feringa, *Chem. Commun.* **56**, 5480–5483 (2020)
[4] E. See, E. Korhonen, M. Nissinen, M. Pettersson, *New J. Chem.* **48**, 21–25 (2024)

Poster 7

Towards Photonic Spin Readout Using Helical Waveguides

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Silicon photonics offers a compelling platform for quantum information processing due to its compatibility with mature fabrication techniques, integrated photonics, and the long coherence times of silicon-based qubits. In this work, we present progress towards a novel system for passive spin readout of photons emitted from quantum sources using helical waveguides. These waveguides, which exploit topological properties, enable the selective coupling of photon polarization states, thus allowing for efficient spin-photon interaction.

Our approach leverages recent advances in topological photonics to achieve robust and loss-resistant transmission, offering a new avenue for scalable quantum information systems. We outline the theoretical framework underpinning our design and demonstrate our experimental progress using scattering-type scanning near-field optical microscopy (s-SNOM) techniques. This method provides high-resolution insights into the photonic structures and aids in optimizing device fabrication.

Our findings suggest that helical waveguides can serve as a powerful tool for passive, on-chip polarization detection, paving the way for enhanced spin readout capabilities in quantum photonic circuits. This work contributes to the ongoing development of silicon-based quantum technology, providing a pathway toward efficient and scalable quantum information processing.

Mammalian Transcription Regulation with Bacterial Two-Component System

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Two-component systems (TCSs) are one of the main regulatory pathways in bacteria. A canonical TCS contains a sensory histidine kinase, which controls the activity of a cognate response regulator protein that usually functions as a DNA-binding transcription regulator. Optogenetics aims to control cell function with light. Our group has developed optogenetic pREDusk tool that utilizes a red light-regulated phytochrome protein [1]. This optogenetic protein acts as a histidine kinase that, through its response regulator, controls gene expression in *Escherichia coli*.

We are currently developing a pioneering optogenetic mammalian transcription tool based on a bacterial TCS. The tool (denoted mREDusk) builds on components from the pREDusk [1] and a blue light-activated mammalian transcription system [2]. We have verified our tool's functionality in human embryonic kidney (HEK 293) cells and are currently modifying it for improved performance. We are also generating mREDusk variants that have inverted activation profile and respond to near-infrared light.

Our mREDusk tool and its variants will be an important addition to the optogenetic toolbox, as bacterial phytochromes have properties especially well-suited for mammalian *in vivo* applications. The absence of systems homologous to bacterial TCS in mammalian cells, also excludes unwanted crosstalk with the host signaling pathways.

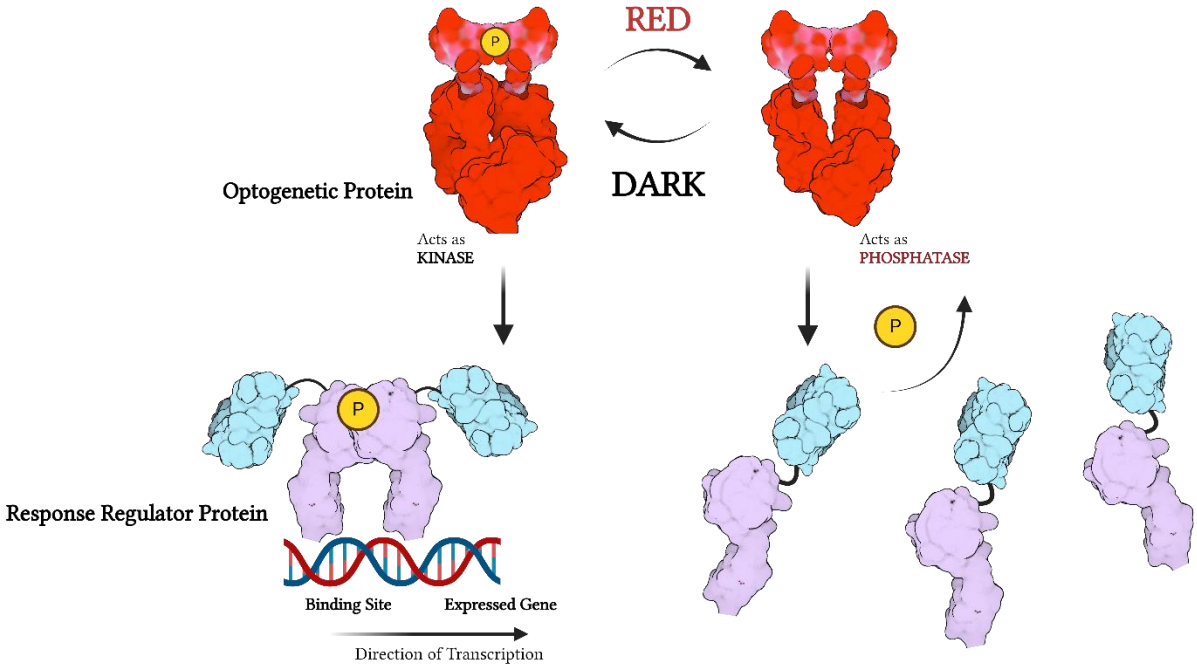

Figure 1: Light-regulated gene expression in mammalian cells with mREDusk tool.

References

[1] Multamäki E, et al. (2022) *Systems and Synthetic Biology*. 11, 3354–3367.
[2] Motta-Mena L, et al. (2014) *Nature chemical biology*. 10, 196-202.

CO_2 Reduction to Methanol at a Cu/Zn–ZrO_2 interface *via* DFT calculations

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A combination of Cu/Zn/ZrO_2 has been found to efficiently catalyse CO_2 conversion to methanol (CTM) [1,2]. It has been suggested that the Cu and Zn components can form a partial alloy under reaction conditions, although this interpretation remains controversial [3,4]. Previous computational studies have mainly focused only on binary systems of Cu–ZnO or Zn–ZrO_2.

We have studied the CTM capabilities of the CZZ system using density functional theory (DFT) calculations and zirconia-supported periodic Cu nanorod models, similar to those in our previous work [5], with some or all interfacial Cu atoms replaced by Zn. A simple kinetic analysis of DFT results was done using the energetic span model [6,7] in order to identify TOF controlling states.

Our results demonstrate that CO_2 hydrogenation intermediates binding to interfacial metal atoms adsorb more strongly to Zn sites than to geometrically equivalent Cu sites at the metal—support interface where the active sites lie. We show that the promoter has little effect on the binding of intermediates which are not in direct contact with the metal component of the system, including some key intermediates identified with the ESM analysis such as the formate and methoxy. Additionally, the results have highlighted the importance of considering hydrogen spillover in computational studies. We show that by including hydrogen spillover, the activation energies for some hydrogenation reaction steps involving zirconia-bound intermediates are much lower than previously reported. These effects lead to an energetic preference for the so-called reverse water—gas shift (RWGS) route of CO_2 hydrogenation (yellow in Fig. 1). Our results therefore help quantify the effect of metallic Zn sites on catalytic properties such as selectivity.

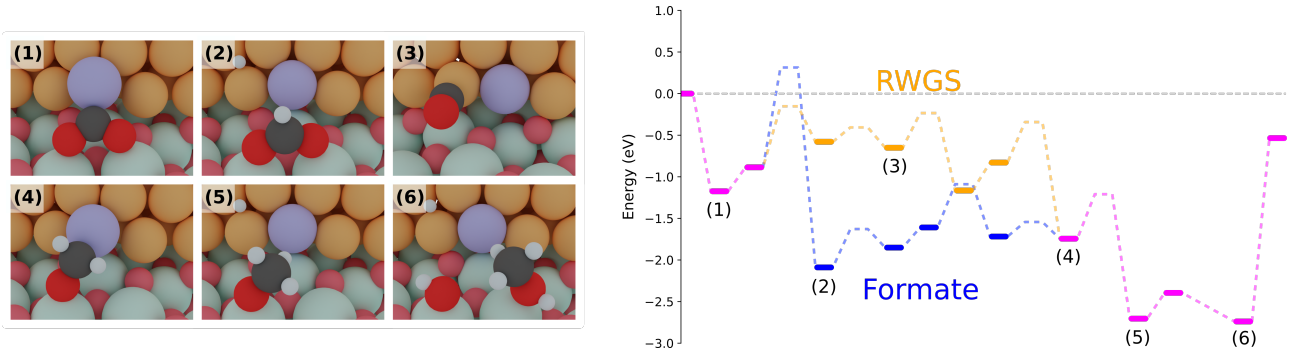

Figure 1: Potential energy surfaces of the RWGS and formate pathways with some key intermediates highlighted.

References

[1] Kattel, S.; Liu, P.; Chen, J.G. J. Am. Chem. Soc. 2017, 139, 9739.

[2] Wang, Y.; Kattel, S.; Gao, W.; Li, K.; Liu, P.; Chen, J.G.; Wang, H. Nat. Commun. 2019, 10, 1166.

[3] Behrens, M.; Studt, F.; Kasatkin, I.; Kühl, S.; Hävecker, M.; Abild-Pedersen, F.; Zander, S.; Girgsdies, F.; Kurr, P.; Kniep, B.-L.; Tovar, M.; Fischer, R.W.; Nørskov J.K.; Schlögl, R. Science 2012, 336, 893.

[4] Nakamura, J.; Fujitani, T.; Kuld, S.; Helveg, S.; Chorkendorff, I.; Sehested, J. Science 2017, 357, eaan8074.

[5] Gell, L.; Lempelto, A.; Kiljunen, T.; Honkala, K. J. Chem. Phys. 2021, 154, 214707.

[6] Kozuch, S.; Shaik, S. Acc. Chem. Res. 2011, 44, 101-110.

[7] Kozuch, S. ACS Catal. 2015, 5, 5242-5255.

ELECTRONIC TRANSPORT IN MULTIWALLED CARBON NANOTUBES

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The electronic transport properties of single multiwalled carbon nanotubes (MWNT) have been intermittently studied since the emergence of carbon nanotubes in the early 90's. The results are still somewhat fragmentary, especially when compared with the successful work performed on single wall carbon nanotubes (SWNT). In practice, the transport properties of a MWNT have mainly been equated with that of the outer layer, as almost without exception the microelectrodes make contact to that one [1]. In high quality MWNTs, the different layers are cleanly separated by the well known van der Waals gap of about 3.4 Å, which significantly limits interlayer interaction.
We have undertaken low temperature conduction measurements on arc-discharge synthesized, semiconducting MWNTs [2]. The diameters of these are in the range 2.5 - 10 nm, that is from just above the size of SWNTs, up to middle sized MWNTs. The energy gap, inversely related to the diameter, varies strongly in this range, and consequently there is a strong dependence of the transport on tube diameter. Certain transport characteristics are much alike those found in SWNT, such as the ON-state resistance and Coulomb blockade. However, the transport gap (Fig. 1) has a more complex behavior than the corresponding one in semiconducting SWNTs, and a number of features, such as negative differential resistance are commonly observed. We present a model for the transport behavior that builds on the possibility of conduction via the second layer.

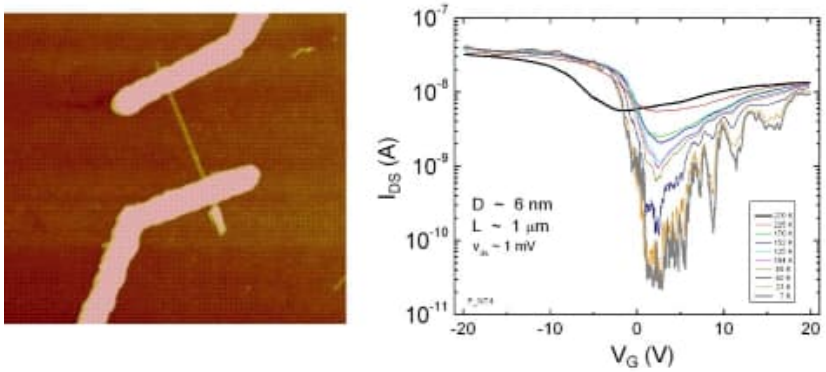

Figure 1: Left: AFM image of MWNT with electrodes Right: Current vs. gate voltage in semiconducting MWNT.

References

[1] D. Mtsuko, A. Koshio, M. Yudasaka, S. Iijima, and M. Ahlskog, Physical Review B. 91, 195426 (**2015**).
[2] M. Ahlskog, O. Herranen, J. Leppäniemi, D. Mtsuko, European Physical Journal B, 95, Nr. 130 (**2022**).

Capillary ordered multiwalled carbon nanotubes as probes of droplet evaporation phenomena

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There is very little investigation of the capillary interaction between individual carbon nanotubes at a fluid interface [1]. We demonstrate capillary interactions on multiwalled carbon nanotubes (MWNT) at the air-water interface and their use for probing the contact line motion of evaporating water droplets. In our experiment, the arc-discharge synthesized MWNTs had typical dimensions with diameters of around 10 nm and lengths at around 1 mm, and were of high quality, but were mixed with graphitic impurity particles in the 10 – 100 nm size range. We used a special technique that distributed the hydrophobic MWNT material on the surface of a spreading water droplet [2]. We observed at the droplet perimeter chain-like structures of end-to-end ordered MWNTs with the graphitic impurity particles attached to the tubes (Fig.1). To explain theoretically the observations at the interface, we investigate the energetics of MWNTs and graphitic impurity particles present in our experimental system. The chains as entities were directed perpendicular to the contact line as a consequence of the contact line behavior upon the subsequent evaporation of the droplet, whereby the contact line was pinned for a relatively long time and the contact angle was continuously reduced. The MWNT chains thus in a unique way probe the local behavior of the contact line.

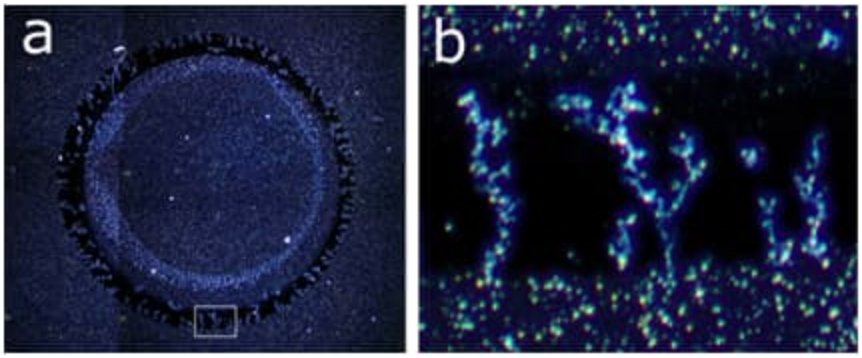

Figure 1. (a) An optical microscope image (size c. 1 mm, stitched together from several images), of a MWNT deposit taken after the experiment, after the droplet has completely dried. See text for closer explanation. (b) A close-up view of the rectangular section in the lower part of the annulus in (a), showing in detail the small chains pointing inwards.

References

[1] T Feng, DA Hoagland, T.P. Russell, Langmuir, **30**, 1072 (**2014**).
[2] MJ Hokkanen et al., Colloids and Surfaces A, **482**, 624 (**2015**).

Poster 12

Evolution of phage resistance through CRISPR adaptation in the mucosal environment

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Keywords: antimicrobial resistance; phage; CRISPR; evolution

Phages, together with other viruses and bacteria, are densely populated on mucosal surfaces, shaping the ecology and molecular diversity of microbial communities. Frequent bacterial exposure to phages have led to the development of various antiviral defense mechanisms, including CRISPR-Cas systems. Although co-evolutionary arms race mostly takes place in the mucosal environment, there is limited data regarding how mucosa impacts phage-bacterium interactions. *Streptococcus mutans* is a significant member of human oral microbiota, and the leading cause of dental caries. To elucidate the effects of mucosal supplementation on phage M102AD infectivity, and natural adaptation of CRISPR-Cas system in *S. mutans* strain P42S, exponentially growing bacterial culture was challenged with phage at two different infection doses (phage-to-bacterium ratio 1 and 100) and plated together with soft agar on solid media with or without mucin (2% w/v) enrichment. After 72h incubation, bacteriophage insensitive mutants (BIMs) were randomly selected from each treatment (72 BIMs in total), purified (3x) before phage resistance profiling and screened with CRISPRloci-PCR on new spacer acquisition. The results showed that infection with higher phage doses was associated with higher phage resistance in *S. mutans* host, while the number of BIMs declined in mucin supplemented conditions, indicating the increased phage virulence in mucosal environment. Interestingly, CRISPR adaptation (i.e. new spacer acquisition) was observed in 55-61% of the BIMs isolated from the mucin treatment groups, while spacer acquisition rate was limited to 22-44% in standard nutrient conditions.
Our data suggests that mucosal milieu directly impacts phage virulence and selection for antiphage defense strategies in *S. mutans* model system, emphasizing the importance of further research on molecular and evolutionary interactions between phages, bacterial hosts and mammalian mucosa.

References:

[1] G. M. de Freitas Almeida, V. Hoikkala, J. Ravantti, N. Rantanen, and L.-R. Sundberg, "Mucin induces CRISPR-Cas defense in an opportunistic pathogen," *Nat Commun*, vol. 13, no. 1, Art. no. 1, Jun. 2022, doi: 10.1038/s41467-022-31330-3.
[2] C. Mosterd and S. Moineau, "Characterization of a Type II-A CRISPR-Cas System in Streptococcus mutans," *mSphere*, vol. 5, no. 3, pp. e00235-20, Jun. 2020, doi: 10.1128/mSphere.00235-20.
[3] L.-R. Sundberg, N. Rantanen, and G. M. De Freitas Almeida, "Mucosal Environment Induces Phage Susceptibility in *Streptococcus mutans*," *PHAGE*, vol. 3, no. 3, pp. 128–135, Sep. 2022, doi: 10.1089/phage.2022.0021.

Sustainable Polydopamine Films via Copper-Induced Oxidation for Energy Storage Applications

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Polydopamine, a multifunctional polymer, has gathered significant attention due to its superior adhesive qualities, biocompatibility, redox activity, and antioxidant properties, all stemming from the oxidative polymerization of dopamine[1]. Despite the potential for wide-ranging applications, conventional synthesis methods often lack scalability, particularly for industrial uses. In this study, we introduce a novel synthesis method driven by metallic copper-induced oxidation, which eliminates the need for chemical oxidants, offering a more environmentally sustainable and controllable process[2].

The polydopamine films produced through this method, in combination with electrospray deposition techniques, exhibit remarkable uniformity and the absence of residual byproducts. Polydopamine contains redox-active monomers such as dopamine-o-quinone, aminochrome, and 5,6-dihydroxyindole, which give it intrinsic electroactivity. These reversible redox transitions in polydopamine films create a pseudocapacitive effect, making them ideal for boosting the energy storage capabilities of supercapacitors [3].

Our findings highlight not only the potential of this synthesis technique for creating biodegradable, efficient energy storage solutions, but also its promise in broader applications such as biodegradable electronics. This work was conducted as part of the EU M-ERA.net InsBIOration project[4], with future research aimed at optimizing electrospray deposition parameters and evaluating the scalability of this process for commercial use.

References

[1] M. d'Ischia, A. Napolitano, A. Pezzella, P. Meredith, T. Sarna, *Angew. Chem. Int. Ed*. 48, **2009**, 3914-3921

[2] M. Al-waeel, J. lukkari, H. Kivelä, M. Salomäki *Langmuir* **2024**, accepted for publication

[3] L. Marttila, M. Salomäki, H. Kivelä, J. Hassinen, S. Granroth, E. Mäkilä, J. Nyman J. Lukkari *ACS Appl. Polym. Mater.* **2023**, 5, 152–164

[4] www.insbioration.de

Micromagnet fabrication and characterization for coupling spins and optomechanics

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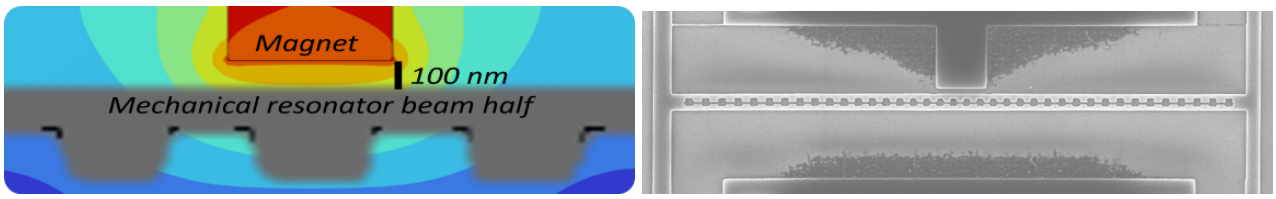
Quantum computing is yet to pass classical computing in speed due to there being too much noise in the system as more and more qubits are added. As such, it is of interest to develop a scalable quantum computing method that can reliably couple multiple qubits. One such avenue is to use an optomechanical system, where donor spin states in silicon are used as qubits. These qubits are coupled to the motion of the mechanical resonator, making the spin state measurable with light. There are multiple advantages to this approach: light is a lossless way of transferring information, donor spins in silicon have been shown to exhibit long coherence times[1] and mechanical motion can be measured more precise than the standard quantum limit [2]. Spin state coupling can be achieved by placing micromagnets near the spins so that the magnetic field gradient experienced by the spins is resonator position dependent (Fig. 1a).

A realisation for this method is yet to be achieved. To prove that this method is a possible solution, we have fabricated samples (Fig. 1b) with micromagnets on a balcony near the resonator and measured the magnetisation with an AFM.



(a) (b)

Figure 1: **a)** A simulation of micromagnet magnetic field gradient. Resonator in grey. **b)** A SEM image of a fabricated sample. A balcony is above the resonator in the picture. No micromagnet on was placed on the balcony.

References

[1] M. Steger et al. “Quantum Information Storage for over 180 s Using Donor Spins in a 28Si ”Semiconductor Vacuum””. In: *Science* 336.6086 (2012), pp. 1280–1283. DOI: 10.1126/ science.1217635. URL: https://www.science.org/doi/abs/10.1126/ science.1217635.

[2] J. D. Teufel et al. “Nanomechanical motion measured with an imprecision below that at the standard quantum limit”. In: *Nature Nanotechnology* 4.12 (Dec. 2009), pp. 820–823. ISSN: 1748-3395. DOI: 10.1038/nnano.2009.343. URL: https://doi.org/10.1038/ nnano.2009.343.

Coherent thermal transport control via pillar-based phononic crystals

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For some time now, phononic crystals (PnCs) have been used to control thermal conductance in insulating and semiconducting materials [1]. At cryogenic temperatures, PnCs have been proposed to be used to improve sensitive infrared detectors and quantum bits. The mechanisms by which PnCs work can be generally divided into two categories: (i) one where incoherent, diffusive, particle-like scattering dominates, and (ii) another where the coherent, wave-like scattering is operational. A large majority of earlier thermal conduction studies have concentrated on geometries where a membrane is perforated by a periodic array of holes. Much less studied are 2D pillar-based PnCs, where the lattice is formed by a periodic array of pillars. For such PnCs, the phonon spectrum can also include localised resonances which cannot carry heat.

In this work, we have fabricated and measured the sub-Kelvin thermal conductance of four pillar-based PnCs with different lattice constants (a) ranging from 300 nm to 5 μm (Fig. 1). We observed a significant reduction in thermal conductance compared to an unaltered membrane, close to an order of magnitude for the $a = 1$ μm PnC. To our knowledge, this is the largest experimentally observed reduction achieved with a pillar-based PnC.

Coherent theory finite element method (FEM), and incoherent theory Monte Carlo simulations were used to compute the thermal conductance of the PnCs. We have also directly measured the phonon dispersion with Brillouin light scattering, the results corresponding to our FEM calculations. For small lattice constants, the experimental thermal conductance qualitatively matches the coherent theory, whereas the larger lattice constants agree with incoherent theory. This is interpreted as a breakdown of coherence, induced by the surface roughness of the pillars.

We have also measured the effect of a magnetic field on the PnCs thermal conductance. By switching the superconductivity of the Al pillars on and off, we can slightly tune the thermal conductance of the structure by affecting the electron-phonon scattering in the pillars.

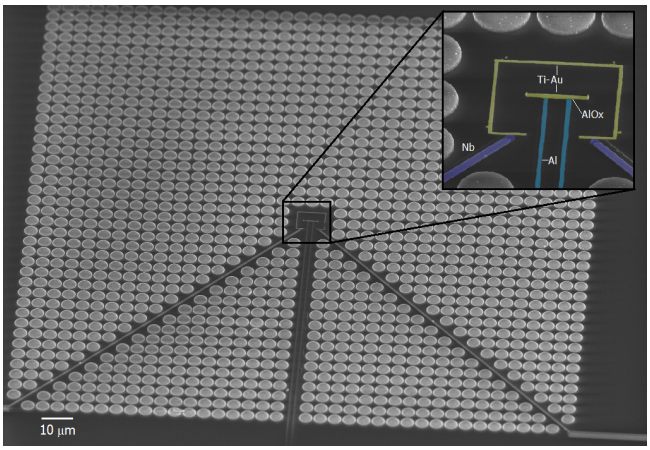

Figure 1: A 5 μm lattice constant Al pillar PnC, with a heater-thermometer structure highlighted in the zoom-in.

References

[1] M. Nomura et al., Mater. Today Phys. ., **22**, 100613 (2022).

Solvent-induced self-assembly of peptide-based systems

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In the gel network, solvents do not typically participate in self-assembly processes. Instead, they are passively encapsulated within the network formed by the gelators. Lately, we have introduced a solvent-induced gelation (SIG) mechanism, where the solvent is chemically active and participates in the formation of organogels, when the self-assembly occurs through the regioselective deprotection of a precursor gelator.[1-2] A key requirement of SIG mechanism is the solvent and precursor gelator to share the same protective group. For instance, the BocFFO*t*Bu precursor gelator is selectively deprotected under acidic conditions in the presence of *tert*-butyl (*t*Bu) acetate solvent. The Boc protected N-terminus of peptide is irreversibly deprotected followed by the reversible deprotection of the *t*Bu-ester at C-terminus due to the hydrolysis of the solvent providing the *t*Bu cation to the system. The reaction pathway forms two gelator molecules which interconvert through a hydrolysis-esterification reaction cycle (Figure 1).[1-3]

The efficacy of SIG self-assembly was assessed on several di- and tripeptide precursor gelators at different solvent environments.[2,3] The concept, based on the general mechanism, extended to peptide precursors with methyl protected C-terminus and solvents bearing the same protective group. In most cases, the solvent-induced self-assembly mechanism was verified, but yielding a different type and extent of assembly was observed.

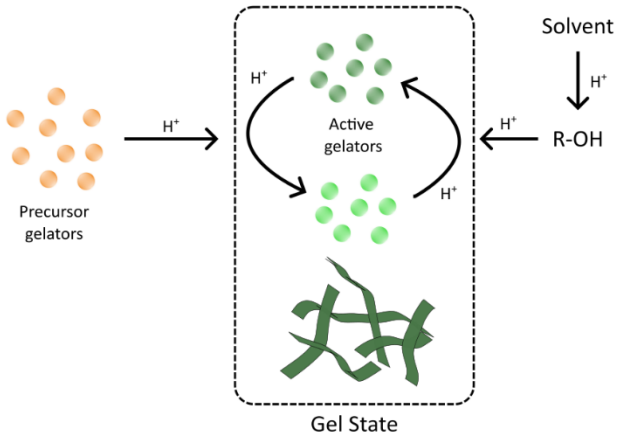

Figure 1: Schematic presentation of solvent-induced gelation mechanism.

References

[1] R. Chevigny, J. Schirmer, Carmen C. Piras, A. Johansson, E. Kalenius, D. K. Smith, M. Pettersson, E. D. Sitsanidis and M. Nissinen, *Chem. Commun.*, **57**, 10375–10378 (2021).

[2] R. Chevigny, H. Rahkola, E. D. Sitsanidis, E. Korhonen, J. R. Hiscock, M. Pettersson and M. Nissinen, *Chem. Mat.*, **36**, 407–416 (2024)

[3] H. Rahkola, E. D. Sitsanidis, R. Chevigny, V. Nikkola, J. Rive, M. Pettersson and M. Nissinen, *manuscript*.

The conformational behavior of peptides with alternating chirality:a first step towards entangled proteins?

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A great variety of molecular scaffolds have been employed to construct foldamers [1] that mimic the secondary structures most commonly found in natural proteins: α-helices and β-sheets.. , In contrast, the possibility to use a native peptide scaffold to generate new types of folds, such as double helices and entanglements, has little been explored [2]. In this work we aim to study the folding behavior of peptides with alternating chirality as a means to access double helical and entangled protein structures. Peptide chirality has been shown to affect their ability to self-assemble [3], and examples of alternating D,L-peptides have been reported to form double helices [4,5]. Our group is currently pursuing two different strategies that use chirality to explore new conformational spaces in peptides. One approach employs a disulfide based dynamic combinatorial system of short homo-and heterochiral peptides to study their assembly behavior. The other approach involves the design of longer peptide strands to form double helix bundles that will subsequently be connected through disulfide bond to form entangled structures.

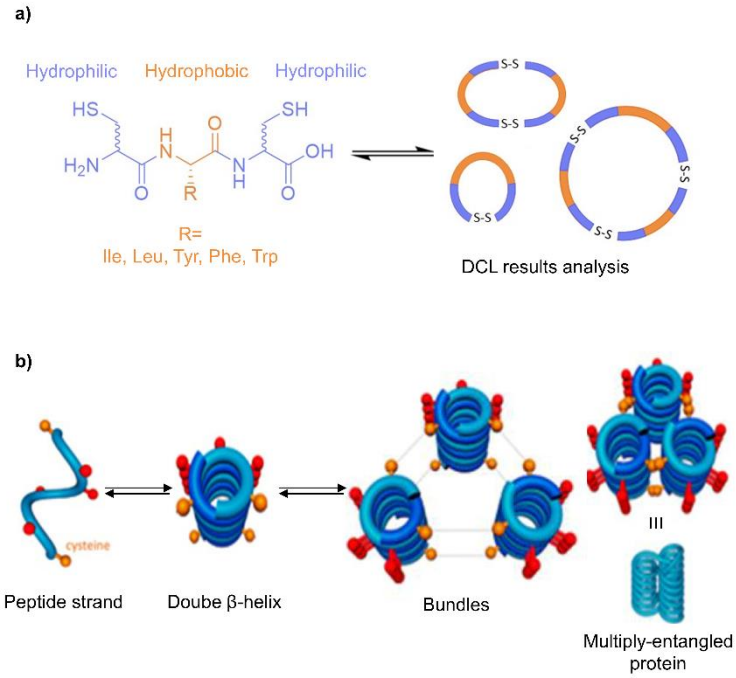

Figure 1: (a) Study of dynamic combinatorial library of peptide with alternating chirality, (b) Strategy to access entangled proteins folds

References

[1] J. Fremaux, C. Venin, L. Mauran, R. H. Zimmer, G. Guichard, S. R. Goudreau, *Nat. Commun.* **10**, 924 (2019).
[2] L.D. Doyle, B. Takushi, R.D. Kibler, L.F. Milles, C.T. Orozco, J.D. Jones, S.E. Jackson, B.L. Stoddard, P. Bradley, *Nat. Commun.* **14**, 6746 (2023).
[3] A.M. Garcia, D. Iglesias, E. Parisi, K.E. Styan, L.J. Waddington, C. Deganutti, R. De Zorzi, M. Grassi, M. Melchionna, A.V. Vargiu, S. Marchesan, *Chem.* **4**, 8 (2018)
[4] B.A. Wallace, *J. Structural Biology*, **121**, 123 (1997)
[5] B. Di Blasio, E. Benedetti, V. Pavone, C. Pedone, C. Gerber, G.P. Lorenzi, *Biopolymers*, **28**, 203 (1989)

Bacteriophage Counteract in vitro-Dysbiosis Induced by Pseudomonas aeruginosa in a Mucosal Environment

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Phages are the most abundant biological entities on Earth and can be found in every environment [1-2]. Recent evidence points out that the impact of phages on life goes beyond the direct infections with their bacterial hosts, reaching a trans-domain evolutionary axis mediated by mucosal and eukaryotic cells interaction [3-8]. The interplay between phages and bacteria often occurs on mucosal surfaces of eucaryotic hosts in a complex environment that has significant implications for homeostasis [9]. The mucus in these tissues segregates phage and bacterial populations, promoting a balance in their co-existence. Beyond physical barrier, mucus is also able to increase bacterial virulence factor expression as well as increasing susceptibility to phage infections [10-11]. This phenomenon suggests that environmental factors might be crucial for development of new phage therapy approaches. The eukaryotic cells and phage interactions might represent important but overlooked biological processes that likely affect dysbiosis control and are crucial for the proper use of phages as antibacterial [12]. Phage therapy is an alternative method to antibiotic treatment that is expanding as a solution to the increasing multidrug-resistant bacteria crisis [13]. Considered an opportunistic bacterium, *P. aeruginosa* is responsible for serious illnesses such as pneumonia and sepsis syndromes, frequently acquiring multidrug-resistant mechanisms [14]. This project aims to understand the role of mucosal environment on phages and eukaryotic cells for control of bacteria-induced dysbiosis by using *P. aeruginosa* as a pathogenic bacteria model. Preliminary results showed that porcine gastric mucin (PGM) treatment affected epithelial cells viability in a bacteria-dependent manner. PGM also enhanced proinflammatory gene expression on those cells, triggered by *P. aeruginosa*. Interestingly, PGM also decreased bacteria internalization in epithelial cells. Pre-incubation with DMS3 phage counteracted the PGM effects on bacteria-infected cells, increasing the eukaryotic cells protection.

References

[1] Clokie *et al.* Bacteriophage. 1(1):31-45 (2011).

[2] Shkoporov *et al.* Cell Host Microbe. 25(2):195-209 (2019).

[3] Almeida *et al.* mBio. 10(6):e01984-19 (2019).

[4] Ellis *et al.* J Biol Chem. 270(35):20717-23 (1995).

[5] Yamaguchi *et al.* J Control Release. 262:232-238 (2017).

[6] Miernikiewicz *et al.* PLoS One. 8(8):e71036 (2013).

[7] van Belleghem *et al.* Sci Rep. 7(1):8004 (2017).

[8] Champagne-Jorgensen *et al.* Trends Microbiol. S0966-842X(23)00146-4 (2023).

[9] Barr *et al.* Proc Natl Acad Sci USA. 110(26):10771-6 (2013).

[10] Almeida *et al.* Microbiol Spectr. 12(8):e0352023 (2024).

[11] Lourenço *et al.* Cell Host Microbe. 28(3):390-401.e5 (2020).

[12] Almeida *et al.* Nat Commun. 13(1):3653 (2022).

[13] Almeida *et al.* Lancet Infect Dis. 20(5):e90-e101 (2020).

[14] Sousa *et al.* Int J Mol Sci. 22(23):12892 (2021).

Carboxylate-catalyzed *C*-silylation of terminal alkynes

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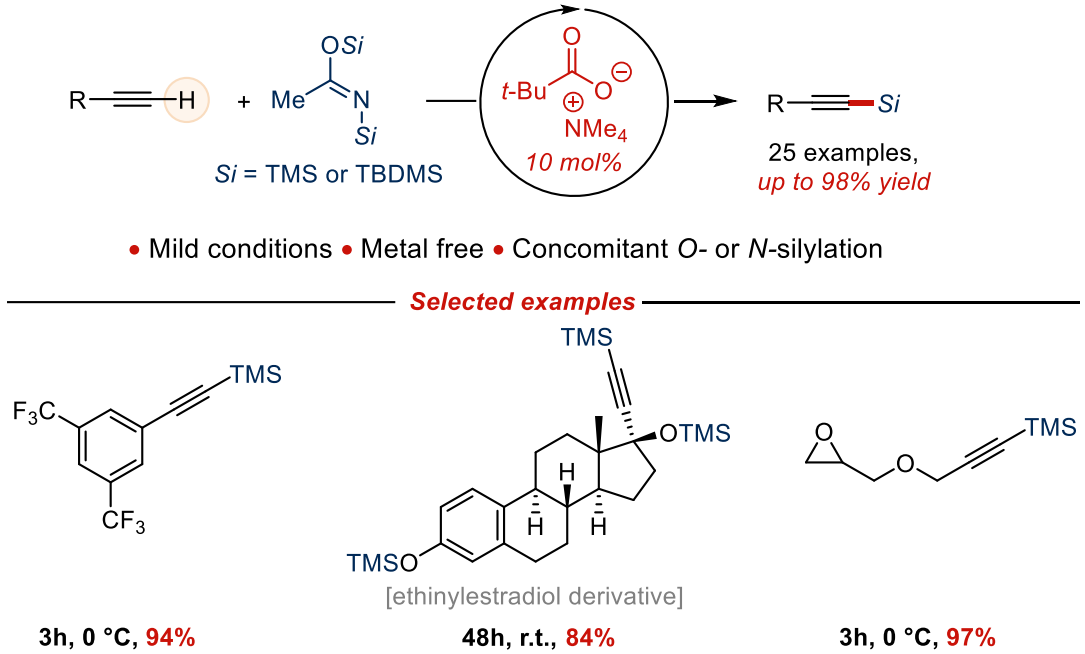
We disclose the bio-inspired application of carboxylate anions in Brønsted base promoted reactions *via* nucleophilic activation of silicon precursors. During our research campaign, we demonstrated mild unconjugated thioester isomerisation catalysed by pivalate anion [1]. Tandem combination of carboxylate anions with *in situ* base releasing reagents, so-called probase reagents, like *N*,*O*-bis-silylacetamide (BSA for trimethylsilyl and BTBSA for *tert*-butyldimethylsilyl) is a novel solution for creating a metal-free strong non-nucleophilic basic system. We implemented that approach in a new rapid diazoaldol reaction protocol with *in situ O*-silylation [2]. To tackle the deprotonation of more challenging substrates we focused on employing terminal alkynes as useful versatile hydrocarbons in reactions with electrophiles. Employing the carboxylate probase combination (here: tetramethylammonium pivalate (TMAP) and BSA or BTBSA), we discovered unprecedented reactivity regarding the formation of *C*-silyl acetylene. The reaction protocol leads to silylacetylene formation hence providing a new way of performing mild trimethylsilyl and *tert*-butyldimethylsilyl protection. With high tolerance to functional groups, a diverse scope of silyl protected acetylenes was obtained under mild metal-free conditions with good to excellent yields (Scheme 1). The comprehensive synthetic exploration of the process, complemented by mechanistic investigation, and plans towards the reactions with other electrophiles will be presented [3].



Scheme 1.

References

[1] S. Riuttamäki, G. Laczkó, Á. Madarász, T. Földes, I. Pápai, A. Bannykh, P. M. Pihko, *Chem. Eur. J.* **28**, (2022).

[2] S. Riuttamäki, A. Bannykh, P. Pihko, *J. Org. Chem.* **88**, 20 (2023).

[3] A. Bannykh and P. Pihko, *Org. Lett.* **26**, 10 (2024).

Exploring the mechanical properties of B_2O_3 glass with classical MD simulations

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Inorganic oxide glasses have numerous applications, and they are used in electronics, healthcare, and as high-strength engineering materials. Glass is considered to be a brittle material, having little to no plastic deformation due to its amorphous structure. Recently, plasticity has been observed in aluminum oxide and densified silica [1,2]. However, little is known about the plastic deformation of boron oxide (B_2O_3) glass. B_2O_3 is a major component in borosilicate glasses, which is why it is important to gain knowledge of its mechanical properties. In this work, it is shown for the first time using molecular dynamics simulations that boron oxide can plastically deform up to 50% tensile strain at room temperature without a fracture. This occurs because of bond switching and the lack of proper three-dimensional structure. B_2O_3 was found to have greater ductility compared to silica, and similar plasticity to aluminum oxide.

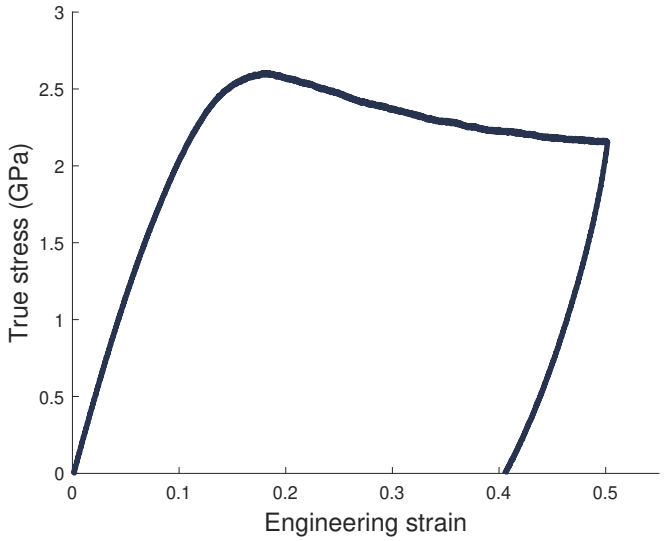

Figure 1: Stress-strain curve of boron oxide glass. No fracture observed up to 50% tensile strain.

References

[1] E. Frankberg *et al.*, *Science* **366** (2019).

[2] J. Zhang, *et al.*, *Acta Materialia* **259** (2023).

STM-induced fluorescent energy transfer between nanomaterials

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Fluorescence energy transfer is the initial step in photosynthesis, where energy is transferred from excited fluorescent donor molecules to surrounding acceptor molecules via Förster resonance energy transfer (FRET), which typically has a maximum transfer distance of 10 nm.[1,2]

We propose a method to exceed this 10 nm limit by bonding donor and acceptor molecules to a molecular bridge through covalent on-surface polymerization. Using a scanning tunneling microscope, we can precisely excite donor molecules via electroluminescence. Additionally, with a plasmon-active tip and optical spectroscopy, we can achieve tip-enhanced electroluminescence to study the fluorescence of single molecules and the energy transfer between them.[2,3,4]

References

[1] *Mirkovic T. et al, Chem. Rev, 117, 249-29*3 (*2017)*
[2] *Luo Y. et al., Nature Communications 15,1677 (2024)*
[3] *Kimouche A. et al, Nature Communications 6*., 10177 (2015)
[4] *Seliverstov A. et al., Surface Science 734, (2023)*

Staphylococcus aureus induces release of IL-1β, IL-18, and active caspase-1 from human retinal pigment epithelial cells

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Staphylococcus aureus (*S. aureus*) can induce endophthalmitis e.g. after surgery, intravitreal injection, or traumatic injury, or be hematogenous in the eye affecting to the retinal pigment epithelium (RPE) causing harm to the retina (e.g. inflammation, retinal detachment, changes in vasculature, edema, or retinal damage and necrosis) [1]. RPE cells are important immune regulators in the retina [2]. *S. aureus* has been shown to induce inflammasome activation in mouse eyes [3]. The inflammasome activation is related to many retinal diseases [4]. In the present study, we exposed human RPE cells to *S. aureus in vitro* and detected the release of inflammasome-related markers.

S. aureus (500 multiplicity of infection [MOI]) and ARPE-19 cells we cultured for 24 h, after which the release of lactate dehydrogenase (LDH) and the secretion of interleukin (IL)-1β (4.5 nm diameter, [5]), IL-18 (5.0 nm diameter, [5]), and active caspase-1 were measured. *S. aureus* induced LDH release and the secretion of IL-β, IL-18, and active caspase-1 into the culture medium when compared to cells without bacteria (Figure 1). *S. aureus* shows high potential to induce inflammasome activation in RPE cells, and further studies are needed to explore the type of inflammasome receptor responsible for this response.

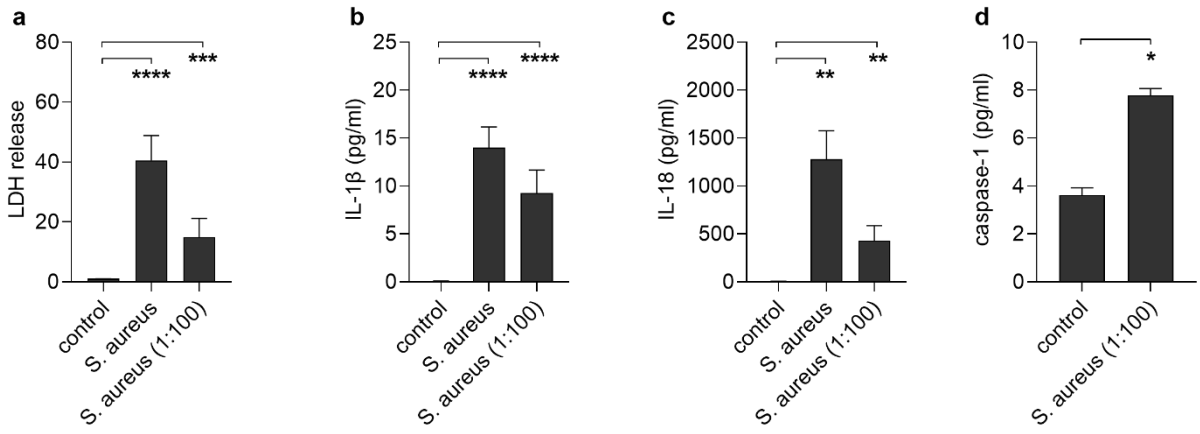

Figure 1: The levels of released LDH (a) and secreted IL-1β (b), IL-18 (c), and active caspase-1 (d) after co-culture of S. aureus and ARPE-19 cells

References

[1.] N. Mahabadi, B. Gurnani, C.N. Czyz. *Treasure Island (FL): StatPearls Publishing* (2024).
[2.] A.W. Taylor, S. Hsu, T.F. Ng. *Front Immunol.* ***12****, 724601 (*2021).
[3.] A. Kumar, P.K. Singh, Z. Ahmed, S. Singh, A. Kumar. *Infect Immun.* **90**, 5 (2022).
[4.] P. Yerramothu, A.K. Vijay, M.D.P. Willcox. *Eye (Lond).* ***32*** (2018).
[5.] B.A. McKenzie, V.M. Dixit, C. Power. *Trends Neurosci.* ***43***, 1 (2020).

Novel Perovskite-inspired Quaternary Mixed-Metal Chalcohalides $M(II)_2M(III)Ch_2X_3$ for Photovoltaic Applications

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Photovoltaic technologies are central to the green transition. New materials are needed to increase power conversion efficiencies, reduce costs, and improve device longevity. The material class of perovskite-inspired quaternary mixed-metal $M(II)_2M(III)Ch_2X_3$ chalcohalides combines the beneficial optoelectronic properties of lead-based halide perovskites with the stability of metal chalcogenides. Lead-free $M(II)_2M(III)Ch_2X_3$ compounds would overcome the stability and toxicity problems of conventional halide perovskites,[1,2,3] and still deliver high conversion efficiencies.[3] Recently, a first single-junction $Sn_2SbS_2I_3$-based solar cell achieved a conversion efficiency of $4.04\,\%$.[3] Materials design and engineering can facilitate the development of $M(II)_2M(III)Ch_2X_3$ compounds to catch up to established photovoltaic technologies.

We utilize density functional theory and machine learning to identify and understand novel $M(II)_2M(III)Ch_2X_3$ compounds, including ns^2 lone pair group IV and V metals for the A-site (Sn, Pb) and for the B-site (Sb, Bi, In), chalcogens for the Ch-position (S, Se, Te), and halogens for the X-position (Cl, Br, I). We computed the energetic stability, the band gap, and the effective electron and hole masses of 54 materials in three phases ($Cmcm$, $Cmc2_1$ and $P2_1/c$; see Figure 1) using PBEsol and the HSE06+SOC hybrid functional.

We identified a total of 22 $M(II)_2M(III)Ch_2X_3$ materials, which fulfill our stability requirements and have a direct band gap in the range of $0.7\,\mathrm{eV}$ to $2.0\,\mathrm{eV}$. Out of the 22, 8 lead-free and 9 lead-based materials are new.[5] For all 54 compounds, $P2_1/c$ is the thermodynamically preferred phase, followed by $Cmc2_1$. Direct band gaps occur predominantly in $Cmcm$ and $Cmc2_1$. Effective e^- masses are larger in $P2_1/c$ than in $Cmcm$ and $Cmc2_1$, whereas effective h^+ masses are similar in all three phases. With machine learning we identify trends across the materials space to formulate chemical rules. The M(III)-Ch bond forms the backbone of $M(II)_2M(III)Ch_2X_3$ compounds. The X-site affects material properties, while the M(II) site allows for fine-tuning.

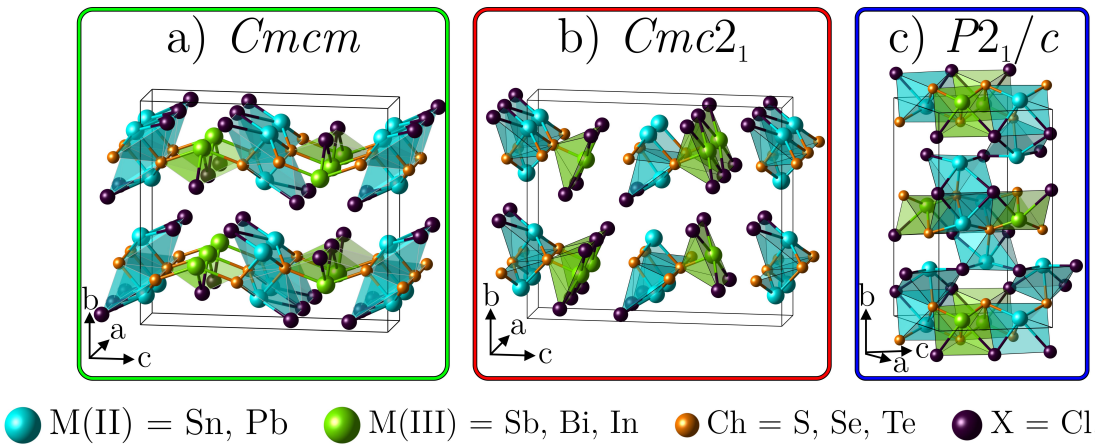

Figure 1: Different phases for $M(II)_2M(III)Ch_2X_3$ compounds [a) $Cmcm$, b) $Cmc2_1$ and c) $P2_1/c$].

References

[1] J. Olivier-Fourcade, *et al.*, Z. Anorg. Allg. Chem. **468**, 91-98 (1980). [2] A. Ibanez, *et al.*, J. Solid State Chem. **55**, 83-91 (1984). [3] V. I. Starosta, *et al.*, Cryst. Res. Technol. **25**, 1439-1442 (1990). [4] R. Nie, *et al.*, Matter **3**, 1701-1713 (2020). [5] P. Henkel, *et al.*, Chem. Mater. **35**, 7761-7769 (2023).

Poster 24

Iron Functionalized Silica Particles as an Ingenious Sorbent for Removal of Fluoride from Water

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The paucity of safe drinking water remains a global concern. Fluoride is a pollutant prevalent in groundwater that has adverse health effects. To resolve this concern, we devised a silica-based defluoridation sorbent from pumice rock obtained from the Paka volcano in Baringo County, Kenya. The alkaline leaching technique was used to extract silica particles from pumice rock, which were subsequently modified with iron to enhance their affinity for fluoride. To assess its efficacy, selected borehole water samples were used. Scanning electron microscopy, X-ray diffraction, Fourier transform infrared and X-ray fluorescence spectroscopy was used to characterize the sorbent. The extracted silica particles were 96.71 % pure and amorphous, whereas the iron-functionalized silica particles contained 93.67 % SiO_2 and 2.93 % Fe_2O_3. The optimal pH, sorbent dose and contact time for defluoridation of a 20 mg/L initial fluoride solution were 6, 1 g and 45 minutes, respectively. Defluoridation followed pseudo-second-order kinetics and fitted Freundlich's isotherm. Fluoride levels in borehole water decreased dramatically; Intex 4.57 to 1.13, Kadokoi 2.46 to 0.54 and Naudo 5.39 to 1.2 mg/L, indicating that the silica-based sorbent developed from low-cost, abundant and locally available pumice rock is efficient for defluoridation.

Keywords: fluoride; sorbent; pumice rock; silica particles; deflouridation

Computational insgihts into the role of tetragonal zirconia in isosynthesis

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Isosynthesis is a catalytic process in which syngas, a mixture of CO and H_2 is transformed selectively to isobutene [1]. The catalyst of choice for this reaction is zirconia (ZrO_2), and more precisely the monolclinic polymorph of zirconia ($m-ZrO_2$). Experimental studies have shown that the product distribution in isosynthesis is particularly sensitive to the polymorph of the catalyst. Namely, tetragonal zirconia ($t-ZrO_2$) is known to produce excess methane instead of the wanted isobutene product [2,3].

In this ongoing computational study, we shed light onto the aforementioned polymorph sensitivity at the atomic scale via DFT+U calculations. The study investigates reaction mechanisms leading to methane formation and C-C coupling on four different zirconia surfaces, that are flat $t-ZrO_2(101)$ and $m-ZrO_2(\bar{1}11)$ structures, and stepped $t-ZrO_2(134)$ and $m-ZrO_2(\bar{2}12)$ structures. In Figure is depicted an example of one investigated elementary reaction, in which methane is produced via hydrogenation of methyl. Using NEB method, transition states have been identified for this and many other related elementary steps, so that the thermodynamics and kinetics of the methane formation on different zirconia surfaces can be compared. In the end, we hope to gain better understanding of how underlying bulk structure (monoclinic/tetragonal) and surface morphology (flat/stepped) affect the syngas reaction network in the context of isosynthesis.

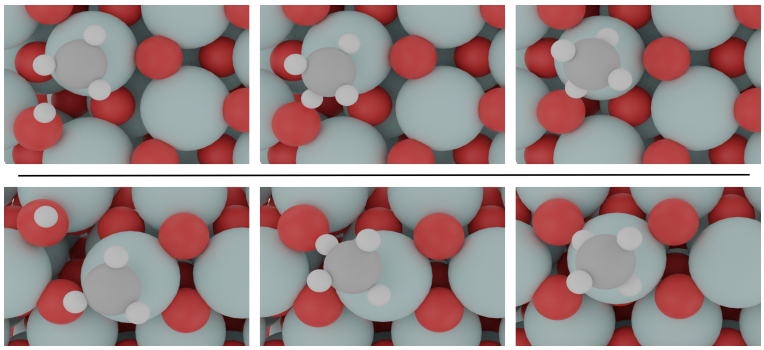

Figure 1: An example of elementary step for methane formation on flat $t-ZrO_2(101)$ (above) and stepped $t-ZrO_2(134)$ (below) surfaces, with transition states found with NEB calculations (middle column).

References

[1] Shah, Y. T. and Perrotta, A. J., Catalysts for Fischer-Tropsch and Isosynthesis, *Product R&D*, **1976**, *15*, 123-131.
[2] Maruya, K., Komiya, T., Okumura, K. and Yashima, M., Linear relationship of the rate of isobutene formation from CO and H_2 on ZrO_2 to the monoclinic phase fraction, *Chem. Lett.*, **1999**, *7*, 575-576.
[3] Wu, X.-m., Tan, M.-h., Geng, H.-l., Zhao, S.-y., Xu, B. and Tan, Y.-s., Effect of crystal structure of ZrO_2 catalyst on isobutene synthesis from CO hydrogenation, *J. Fuel Chem. Technol.*, **2023**, *51*, 473-481.

Microplastics in Kenya: Assessing the Efficacy of Removal of Microplastics in Conventional and Membrane Bioreactor Wastewater Treatment Plants.

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In Kenya, plastic waste represents 20% of the total solid waste generated; around 22,000 tonnes of solid waste is generated daily, with per capita consumption of plastic estimated at 0.03 kg, totaling 0.5 to 1.3 million tonnes of plastic waste annually[1]. Despite these huge volumes, only 8% of the plastic is recycled; the rest is majorly landfilled or incinerated (also burnt) or disposed onto surface waterways. Plastic waste in the environment undergoes mechanical, chemical, and biological degradation, resulting in microplastics (particles ≤5 mm), including fragments, fibers, foams, spheres, and films. These particles are resistant to further breakdown, bioaccumulate, and are dispersed by wind and ocean currents. Microplastics are emerging as a global environmental threat, particularly in aquatic ecosystems. Despite the ban on single-use plastics in Kenya, the presence of microplastics remains significant and their impact on the ecosystem is largely unknown and not quantified. Research conducted along Kenya's coast and in Lake Naivasha highlights substantial microplastic contamination. Common microplastic types found included fragments, fibers, and films, predominantly composed of polypropylene, polyethylene, and polyester. Coastal studies identified 149 microplastic particles with concentrations ranging from 33.3 to 275 particles/m³, increasing with distance from land. In Lake Naivasha, surface water microplastic concentrations ranged from 0.183 to 0.633 particles/m².[2,3] Our continuing study examines the presence and characterization of microplastics in sludge from wastewater treatment plants (WWTP), which are significant point sources of microplastic pollution. Analysis microplastics in sludge samples from WWTPs (conventional and membrane bioreactor) in Nairobi was done after enzyme digestion using Raman spectroscopy. Conventional plants showed an average of 321 ± 80.92 particles per 25 g of sludge, while membrane bioreactor plants had 556 ± 29.77 particles. Fragments accounted for 53% of the microplastics, followed by fibers at 20%, with an average particle size of 53 µm. Statistical analysis (t-test, P = 0.146) revealed a significant difference in microplastic removal efficiency between the two WWT methods. These findings highlight the urgent need for improved waste management strategies and further research to address microplastic pollution in Kenya's aquatic systems.

References

1 https://kpp.or.ke/2022/08/29/roadmap-to-2030-kenya-plastics-pact-releases-its-national-strategy/
2 https://doi.org/10.1016/j.marpolbul.2022.113710
3 https://doi.org/10.1002/etc.4677

Keywords: microplastics, wastewater treatment plant, sludge, Raman spectroscopy

Synthetic Strategies and Preliminary Studies of Mono- and Dinuclear Complexes with Potential Opto-magnetic Properties

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The seminal work that reported magnetic properties of a dysprossocenium $DyCp_2$ (Cp = cyclopendienyl) system at 60 K, stimulated the interest in single-molecule magnets (SMM)[1]. Since then, considerable efforts in the field produced a wide variety of monometallic lanthanide ions based on Cp ligands. Even simple structures with a straightforward synthesis have demonstrated to have well-defined, highly tuneable properties[2]. At the same time, the high impact achieved by the mononuclear systems, led as well to an increase in coupling two magnetic centres to obtain bimetallic structures. For instance, connecting two lanthanide fragments through a (radical) bridging ligand can enhance the molecular magnetism, but also provide photonic properties[3].

Based on previous works carried out by our research group, we are investigating both mono- and bimetallic lanthanide SMMs. On the one hand, we are working on expanding the homo- and heteroleptic cyclopentadienyl monometallic systems, by combining alkyl and aryl substituents to yield complexes type $LnCp_2$ or $LnCp_2(E_2R)$ (E = O, S, N), and on the other, we are also exploring the possibilities of bimetallic bridged systems closely related to tetraoxolene type.

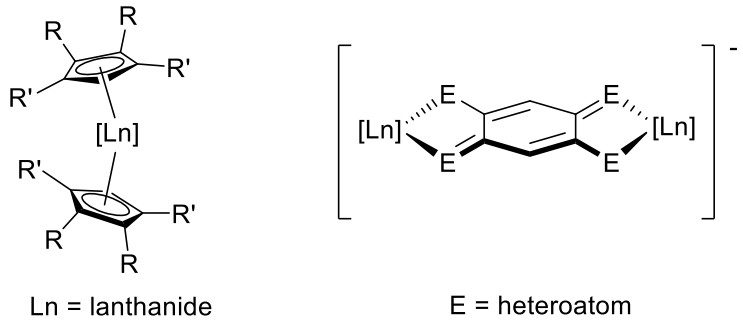

Figure 1: Some of the systems currently investigated by our group.

References

[1] a) C. Goodwin, F. Ortu, D. Reta, N. Chilton, D. Mills. *Nature* **548**, 439 (2017) b) F.-S. Guo, B. M. Day, Y.-C. Chen, M.-L. Tong, A. Mansikkamäki, R. Layfield. *Angew. Chem. Int. Ed.* **56**, 11445 (2017)

[2] A. Zabala-Lekuona, J. M. Seco, E. Colacio. *Coord. Chem. Rev.* **441**, 213984 (2021)

[3] a) S. Demir, J. M. Zadrozny, M. Nippe, J. R. Long. *J. Am. Chem. Soc.* **134**, 45, 18546 (2012); b) D. Errulat, R. Marin, D. A. Galico, K. L. M. Harriman, A. Pialat, B. Gabidullin, F. Iikawa, O. D. D. Couto, J. O. Moilanen, E. Hemmer, F. A. Sigoli, M. Murugesu, M. *ACS Cent. Sci.* **5**, 7, 1187 (2019)

Relocalization of the host Ki-67 during parvovirus infection promotes the nuclear egress of progeny capsids

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Canine parvovirus (CPV) is a small DNA virus that uses the host cell nucleus as the replication site. Expansion of the replication compartment is accompanied by dramatic alterations in host chromatin architecture, resulting in a condensed chromatin layer at the nuclear periphery. Our recent BioID study identified the nucleolar protein Ki-67 as an interactor of the parvoviral non-structural protein 2 (NS2) [1]. Ki-67 is a chromatin-associated protein, which relocalizes to mitotic chromosomes and organizes the perichromosomal sheath. During CPV infection, we observed a shift in Ki-67 localization from nucleoli to nucleoplasm, as well as a significant increase in nuclear Ki-67 intensity and correlation with DNA as the infection progressed. Here, we further verified the association of NS2 and Ki-67 by quantitative immunofluorescence microscopy and proximity ligation assay. Overexpression of NS2-EGFP lead to a prominent cytoplasmic relocalization of Ki-67, whereas this effect was not seen in cells overexpressing the larger non-structural viral protein NS1-EYFP. In infection, the nucleoplasmic distribution of Ki-67 was associated with an increase in the nuclear egress of progeny capsids. Notably, nucleoplasmic Ki-67 distribution was not detected in infected cells lacking full-length NS2, and the nuclear egress of capsids was reduced. Our findings suggest that viral NS2 is involved in the nucleoplasmic redistribution of Ki-67, which results in an altered nuclear environment promoting the pre-lytic nuclear egress of viral capsids.

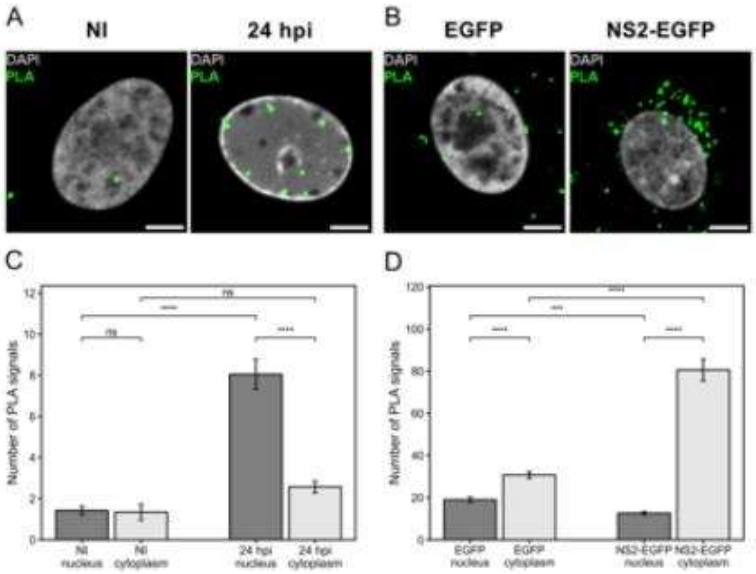

Figure 1: NS2 is associated with Ki-67 as shown by proximity ligation assay.

References

[1] S. Mattola, *et al.*, *PLoS Pathog*. **18**, 4 (2022).

Fabrication of self-supporting thin film lithium niobate platforms separated by a submicron gap

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Heat transfer mechanisms in classical physics are mainly considered to be convection, conduction and radiation. Of the three, only radiation is capable of transferring heat between two bodies in a vacuum without any contact. Specifically, heat radiation, as considered in classical physics, is more accurately known as as far-field radiative heat transfer, where heat is transferred by propagating photons. The more precise name is important because, on the microscopic scale, near-field radiative heat transfer (NFRHT) begins to dominate. Near-field radiation is enabled by photon tunneling between two bodies, and transfer of heat flux can be orders of magnitude higher than in the far-field case if the gap between the two bodies is smaller than the dominant photon wavelength. NFHRT can be used in many applications, with the the most obvious one is contactless cooling, which has already been demonstrated [1].

Another strong contactless heat transfer mechanism arises from tunneling acoustic phonons. Acoustic phonons are the quanta of mechanical vibrations in solids and are the dominant heat carriers in dielectric solids. Contrary to common belief, it has been demonstrated theoretically [2] that phonons in piezoelectric materials can tunnel across short distances over a vacuum, assisted by the piezoelectric response. This piezoelectrically mediated heat transfer (PEHMT) has even been shown to be the dominant transfer mechanism for piezoelectric materials at low enough temperatures and small distances [3], and PEHMT has also been demonstrated experimentally [4].

The fabrication of free-standing thin membrane platforms was investigated using lithium niobate to further study acoustic phonon tunneling with piezoelectrically stronger material than AlN used in earlier experiments [4]. These platforms were separated by a submicron gap using industry-standard lithium-niobate-on-insulator (LNOI) silicon chips. The platforms were realised by dry etching the $LiNbO_3$ (lithium niobate) layer to outline the platforms and then released by vapor etching the SiO_2 layer with HF vapor from underneath the $LiNbO_3$ layer. A three-layer etch mask of mr-PosEBR 0.3 - Al_2O_3 - Cr was utilised in $LiNbO_3$ dry etching to achieve good gap edge quality. An estimated Cr to $LiNbO_3$ selectivity of 0.3 was achieved with an estimated $LiNbO_3$ etch rate of 6 nm/min and edge wall verticality of $56°$.

References

[1] Linxiao Zhu et al. In: *Nature* 566.7743 (Feb. 2019), pp. 239–244.

[2] Zhuoran Geng and Ilari J. Maasilta. In: *Phys. Rev. Res.* 4 (3 June 2022), p. 033073.

[3] Zhuoran Geng and Ilari J. Maasilta. 2023. arXiv: 2303.05084[cond-mat.mes-hall].

[4] Zhuoran Geng. PhD thesis. University of Jyväskylä, 2023. ISBN: 978-951-39-9533-1.

Poster 30

Activating the Innate Immunity System to fight against microbial infections

IN-ARMOR -project

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Antimicrobial resistance (AMR) is recognized by the World Health Organization (WHO) as one of the most significant threats to global food production and health care [1]. The widespread use of antibiotics has exacerbated AMR, leading to the emergence of bacterial strains and fungi that can cause infections even in individuals with normal health. AMR poses a severe danger to those who have low immune systems, such as young children and older adults. There is a critical shortage of antimicrobials, particularly new protocols for developing and producing cost-effective treatments. The In-Armor project investigates novel methods for synthesizing aroylated phenylenediamines (APDs) using computer-aided drug design and in-silico approaches [2]. These APDs are designed to activate antimicrobial peptides (AMPs), thereby enhancing innate immunity and inhibiting histone deacetylases [2]. The reference compound used in this study is Entinostat [2,3]. Human cells are exposed to APD compounds to evaluate the effects of the designated APDs. Innate immunity activation is followed, and the effects are observed under AMR bacterial, fungal, and viral infections. At the University of Jyväskylä, bacterial and viral infections are studied when collaborators examine the effects against fungi. Nine Universities research institutions are collaborating with seven medical industry partners to target the goal, of finding new methods and compounds to fight against AMR. The consortium that walks through this project collects people from 10 countries in the EU Iceland (leader of the project), Sweden, Spain, Finland, France, Netherlands, Belgium, Ukraine, Czechia, and Germany. Comprehensive details and additional information regarding this project are available on the official website: https://inarmor-project.eu/. This project is funded by the European Union´s Horizon Europe research and innovation program under grant agreement No 101080889.

References

[1] Antimicrobial Resistance Collaborators. (2022). Global burden of bacterial antimicrobial resistance in 2019: a systematic analysis. The Lancet; 399(10325): P629-655. DOI: https://doi.org/10.1016/S0140-6736(21)02724-0

[2] Bergman P, Raqib R, Rekha RS, Agerberth B, Gudmundsson GH. Host Directed Therapy Against Infection by Boosting Innate Immunity. Front Immunol. 2020 Jun 12;11:1209. doi: 10.3389/fimmu.2020.01209. PMID: 32595649; PMCID: PMC7304486.

[3] Connolly RM, Rudek MA, Piekarz R. Entinostat: a promising treatment option for patients with advanced breast cancer. Future Oncol. 2017 Jun;13(13):1137-1148. doi: 10.2217/fon-2016-0526. Epub 2017 Mar 9. PMID: 28326839; PMCID: PMC5618943.

Metal–ligand bond in group-11 complexes and nanoclusters

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Comprehension chemical nature of bonds in metal-ligand complexes and nanoclusters, which arises from the innate properties of the building components, facilitates understanding of probable reactions and aiding to learn and develop novel synthesis procedures. However, there is a paradox due to the critical and unknown properties of the materials. Our study focuses on geometric, energetic, and electronic properties of metal-ligand bonds in a series of group-11 metal (Cu, Ag, Au) complexes as M-L and ligand-protected metal nanoclusters denoted as $[M_{13}L_6Br_6]^-$ using various ligand groups including thiolates, phosphine, alkynyls, and N-heterocyclic carbenes (NHCs) [1].

All calculations have been done by using DFT as implemented in the real-space code package GPAW (Grid-based projector-augmented wave method) [2]. The study provides calculations using PBE [3] and BEEF-vdW [4] functionals. This work has summarized the relevance of understanding the characteristics of the metals, and the effect of the metal d-band on binding properties. The study underlines gold's pivotal role in forming stable metal-ligand complexes and nanoclusters, but is questioning its role as an only decisive option. This study showed the order $Ag - L > Au - L > Cu - L$ for bond lengths in metal-ligand complexes. Moreover, the copper clusters, possessing the shortest average M-L bonds, exhibit the second-highest binding energies following gold clusters. By analyzing the projected density of states and molecular orbitals in complexes and clusters, the M-thiolate bonds were shown to have σ and π bond characteristics whereas phosphines and carbenes were creating σ bonds to the transition metals. This study suggests that PPh_3 and NHCs-protected Cu clusters are most stable after Au clusters. Moreover, it implies that using a combination of metals and ligands can lead to improved binding affinities and versatile surface motifs. The findings demonstrate the significant role of copper in potentially advancing the metal-ligand interface in protected nanoclusters, contributing to the development of new materials which can open a new avenue for applications like highly selective catalysis.

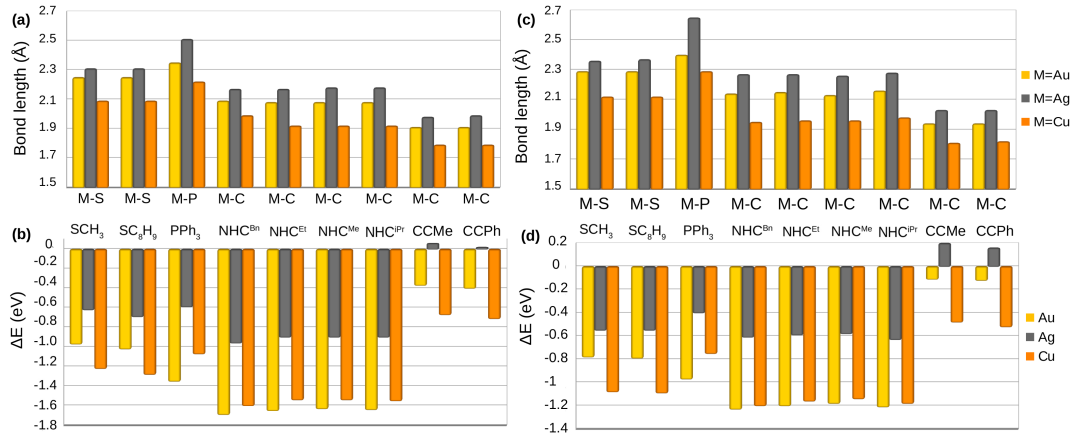

Figure 1: Bond length M-L (Å) and binding energy (eV) calculated by PBE (shown in (a) and (b)) and BEEF-vdW (shown in (c) and (d)) for the M-L complexes.

References

[1] M. Sabooni Asre Hazer, S. Malola, and H. Häkkinen, *Phys. Chem. Chem. Phys.* **26**, 21954-21964 (2024).

[2] J. Enkovaara, et al., *J. Phys.: Condens.Matter* **22**, 253202 (2010).

[3] J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* **77**, 3865 (1996).

[4] J. Wellendorff, et al., *Phys. Rev. B: Condens.Matter Mater. Phys.*, **85**, 235149 (2012).

Functional properties of Finnish berries

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Natural biomaterials have been important in Finland's bioeconomy. Finland has a particularly abundant supply of berry resources. Many berries are used in foods, cosmetics, and the pharmaceutical industry. Wild berries are cherished by local people. Berries' functional properties such as antioxidant, anti-inflammatory, anticancer, and more have been studied over the years [1], [2]. However, there is still much room for research on antibacterial and antiviral properties. Additionally, some wild berries which have bitter taste are often overlooked and not consumed. In this study, we conduct comprehensive antiviral and antibacterial screening on approximately 20 different wild and cultivated berries (Figure 1). We aim to discover new values in both overlooked berries and commonly consumed berries.

Figure 1: The wild and cultivated berries we have collected so far.

	Berry	scientific name		Berry	scientific name		Berry	scientific name
1	Rowanberry	*Sorbus aucuparia*	7	Raspberry (cultivated)	*Rubus idaeus*	13	Red gooseberry	*Ribes uva-crispa*
2	Lingonberry	*Vaccinium vitis-idaea*	8	Blackcurrant	*Ribes nigrum*	14	Blueberry "North blue"	*Vaccinium angustifolium*
3	Cloudberry	*Rubus chamaemorus*	9	Strawberry "Jonsok"	*Fragaria x ananassa Duchesne*	15	White rowanberry	*Sorbus koehneana*
4	Bilberry	*Vaccinium myrtillus*	10	Strawberry "Sonsation"	*Fragaria x ananassa*	16	Chokeberry (Jyväskylä)	*Aronia mitschurinii*
5	Raspberry (wild)	*Rubus idaeus*	11	Red currant (Pori)	*Ribes rubrum*	17	White currant	*Ribes rubrum*
6	Chokeberry (Mikkeli)	*Aronia mitschurinii*	12	Red currant (Kangasniemi)	*Ribes rubrum*	18	Crowberry	*Empetrum nigrum*

References

[1] B. Baby, P. Antony, and R. Vijayan, "Antioxidant and anticancer properties of berries," *Crit. Rev. Food Sci. Nutr.*, vol. 58, no. 15, pp. 2491–2507, Oct. 2018, doi: 10.1080/10408398.2017.1329198.

[2] N. Pap *et al.*, "Berry polyphenols and human health: evidence of antioxidant, anti-inflammatory, microbiota modulation, and cell-protecting effects," *Curr. Opin. Food Sci.*, vol. 42, pp. 167–186, Dec. 2021, doi: 10.1016/j.cofs.2021.06.003.

Fabrication of quantum devices with helium ion beam direct writing

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Quantum devices are typically fabricated by depositing different materials in several complex fabrication steps. Here we take a different approach and demonstrate fabrication of complete quantum devices using a single superconducting film and only few fabrication steps. To achieve this, we use helium ion beam direct writing [1], to fabricate Josephson junctions for quantum devices. In the direct writing method, superconductivity is suppressed locally via disorder induced by the focused helium ion beam in a helium ion microscope (HIM), thus creating a weak link to serve as a Josephson junction. As the strength of the weak link can be tuned continuously from superconducting to insulating, this method enables exceptionally good control over the weak link properties. The method was first demonstrated in YBCO [1], and here we extend this method to NbTiN [2], which is more suitable material for quantum device applications. We grow NbTiN films epitaxially using pulsed laser deposition (PLD)[3,4], with the deposited films having excellent electrical characteristics and Tc reaching as high as $\sim$16 K. Transport measurements of the Josephson junctions formed with the direct writing method show good characteristics in both DC and under microwave illumination, indicating that they are suitable for use in wide range of devices [2]. With this method, we can fabricate both SNS and SIS type of devices and control the critical current density by five orders of magnitude allowing specific tailoring of junction properties for each application. As an example, we demonstrate the successful fabrication of high-quality superconducting quantum interference devices (SQUIDS) using the direct writing method. These devices have good performance and flux noise approaching the state-of-the-art.

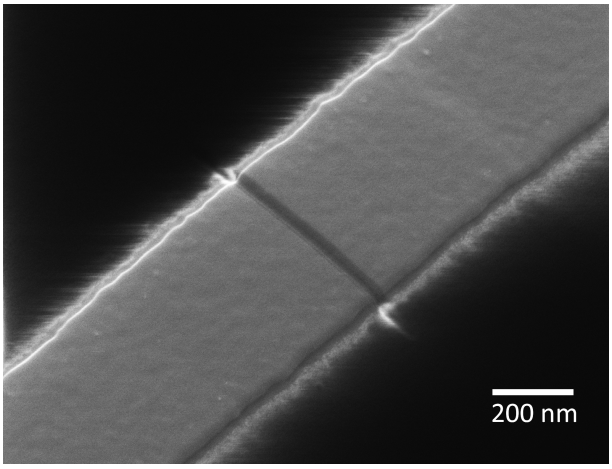

Figure 1: Helium ion microscope (HIM) image of a Josephson junction fabricated with direct writing.

References

[1] S. Cybart, E. Cho, T. Wong, et al., *Nat. Nanotechnol* 10, 598–602 (2015)
[2] A. Ruhtinas and I. J. Maasilta, *arXiv:2303.17348v2* (2024)
[3] S. Chaudhuri, M. R. Nevala, et al., *IEEE Trans. Appl. Supercond.*, 21(3), 143-146 (2011).
[4] A. Torgovkin, S. Chaudhuri, et al., *Supercond. Sci. Technol.*, 10(5), 055017 (2018).

Nucleus softens during herpesvirus infection

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Mechanical properties of the nucleus are remodeled not only by extracellular forces transmitted to the nucleus but also by internal modifications, such as those induced by viral infection. During herpes simplex virus type 1 infection, the viral regulation of essential nuclear functions and growth of nuclear viral replication compartments are known to reorganize nuclear structures. However, little is known about how infection-induced nuclear deformation changes nuclear mechanobiology. Our analyses show that the nuclear center has a low-density viral replication compartment. The nuclear volume, height, and nuclear envelope tension are increased. While the amount of lamin proteins increases, the nanoscale motion of the nuclear lamina is reduced, and the LINC complex protein, SUN2, is strongly downregulated. The combined effect of these various nuclear changes leads to nuclear softening. The computational modeling of virus-induced changes in cellular forces showed that increased nuclear volume and height increased the nuclear stiffness. In contrast, the removal of lamina-associated domains of the chromatin led to significant nuclear softening. The decrease in outward forces, such as reduced intranuclear osmotic pressure and cytoskeletal pull, strongly decreased nuclear stiffness. A change in chromatin viscosity had a smaller effect, and the known infection-induced disintegration of the nuclear lamina reduced stiffness only when outward forces were low. The simulations showed that an increase in the nuclear envelope tension can occur with a decrease in nuclear stiffness. Based on these findings, we propose a mechanical model that explains mechanistic coordination between the nuclear deformation in infection and decreased nuclear stiffness.

Poster 35

Plasmonic enhancement of circular dichroism

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In everyday life, we perceive chirality (the different handedness of molecules) through different smells, tastes, or different effects on our bodies associated with enantiomers (a pair of chiral molecules). The differences, e.g., in distribution and metabolism of enantiomers can have severe implications for people [1] and the environment [2]. The chirality of molecules may determine whether a drug achieves its desired beneficial effect or becomes toxic [1]. The degradation of chiral chemicals in the environment and wastewater treatment plants can be enantioselective, which can lead to an accumulation of chiral environmental toxins [2]. It is therefore important to be able to detect molecular chirality in pharmaceuticals and wastewater to avoid or counteract environmental issues. Circular dichroism (CD) spectroscopy exploits the different absorption of left- and right-handed circularly polarized light by chiral molecules [3] and can be used to discriminate enantiomers. The applicability of CD spectroscopy is currently limited by the fact that CD signals are often weak and difficult to detect [4]. The interaction of plasmonic nanoparticles (NPs) with chiral molecules is a promising approach to amplify weak chiral signals but lacks predictive computational frameworks. This poster presents our systematic study for a predictive characterization of plasmonic CD enhancement. Sets of different organic molecules and metal nanoparticles will be used to identify the main dependencies of plasmonic CD enhancement. Our characterization bases on first principles calculations with time-dependent density functional theory. Most likely structures of the molecules on the nanoparticles are obtained using a machine learning code called Bayesian Optimization Structure Search [5]. Identified dependencies of plasmonic CD enhancement will be used in a theory-experiment NP-design study, which will comprise different materials, geometries and dimers. Codes for obtaining optimized NPs for CD enhancement that can be used in research and industry will be

Characterization of surface-grafted polymer nanobrushes by Infrared Scanning Near-Field Optical Microscopy

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Surface-grafted polymer brushes are thin polymer coatings that provide new properties to modified surfaces. They consist of densely packed polymer chains tethered at one end to a solid substrate. Due to their high grafting density, the macromolecules adopt extended conformation – such highly-oriented structure distinguishes them from other polymeric nanocoatings. Polymer brushes have found various applications in biomedicine, e.g., for fabrication sensors, drug delivery systems, antibacterial and antifouling coatings, in environmental technologies as high-performance lubricants or wastewater treatment devices, and in electronics for photovoltaic systems or organic electronics [1].

Scattering-type Scanning Near-field Optical Microscopy (sSNOM) operating in infrared wavelengths is a perfect technique for characterizing polymer brushes, as it provides detailed chemical and morphological information [2]. Infrared absorption maps are used to confirm the spatial distribution of functional groups and successful post-polymerization modification that is crucial in the synthesis of advanced materials. Additionally, topography images provide information about the thickness of synthesized polymer brushes and the homogeneity of the coating.

In this study, poly(methacrylic acid) brushes were synthesized on SiO_2 substrate by surface-initiated organocatalyzed atom transfer radical polymerization. The study involved synthesizing homogeneous layers and patterned brushes. These brushes were characterized using sSNOM at selected wavelengths to investigate spatial control over the polymerization and the distribution of functional groups.

Acknowledgements

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References

[1] A. Kiełbasa, K. Kowalczyk, K. Chajec-Gierczak, J. Bała, and S. Zapotoczny. *Polymers for Advanced Technologies*, **35(4)**, e6397 (2024).

[2] K. Wolski, J. Smenda, A. Grobelny, P. Dąbczyński, M. Marzec, A. Cernescu, M. Wytrwal, A. Bernasik, J. Rysz, and S. Zapotoczny. *Journal of Colloid and Interface Science*, **634**, 209-220 (2023).

NMR spectroscopy as a versatile tool for studying intrinsically disordered proteins and mechanism of antimicrobial resistance

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Nuclear magnetic resonance (NMR) spectroscopy stands unique among biophysical tools as it delivers dynamics embedded to atomic-level details of structure and interactions. Spatio-temporal resolution of NMR can be employed to address bewildering myriad of biological questions. Our Lab develops and applies NMR methodology together with other biochemical and biophysical tools to study structural and functional properties of intrinsically disordered proteins/regions (IDPs/IDRs) as well as to understand synthesis and maintenance of bacterial cell wall in staphylococcaceae [1,2].

IDPs/IDRs are polypeptides devoid of well-defined, stable 3D structure, yet displaying functional importance. Thus, they go against structure defines function paradigm that is an integral part of structural biology. IDPs/IDRs are notoriously difficult to study due to rapid interconversion between different conformers and conformational states. However, spatio-temporal resolution of NMR spectroscopy paves the road for understanding their mechanistic properties driving the function [1].

Our cell homeostasis is maintained by highly fine-tuned and regulated interactions driven by short linear motifs (SLiMs) embedded into IDRs of cellular proteins. Many bacteria encode for specific secretion systems to deliver effector proteins into host cell. By mimicking cellular SLiMs these effector proteins can acquire higher affinity and excel in the case of competitive binding with host proteins. One example of such bacterial effector protein is enterohemorrhagic *E. coli* (EHEC) $EspF_U$, and its close relative EspF, predominantly found in enteropathogenic *E. coli* (EPEC). Both are secreted bacterial effectors with several highly conserved proline-rich repeats of 47 residues injected to intestinal epithelial cells through type 3 secretion system (T3SS) and target the GTPase binding domain (GBD) of neural Wiskott-Aldrich syndrome protein (N-WASP). However, their SH3 binding motifs target different proteins, sorting nexin (SNX) 9 in the case of EspF and Insulin receptor tyrosine kinase substrate (IRTKS) in the case of $EspF_U$ [3,4]. We characterized the free form of a single-repeat EspF and its complex forms with SNX9 SH3 and N-WASP GBD as well as the trimeric complex. We also evaluated the thermodynamics of EspF binding to its target proteins and studied the disruption of the autoinhibitory state of N-WASP GBD by EspF [4].

Antimicrobial resistance (AMR) poses a serious threat to our health and economy. *S. aureus* is a Gram-positive bacterium and its notorious methicillin- and vancomycin-, the drug-of-last-resort, resistant *S. aureus* strains MRSA and VRSA establish a slow pandemic associated to high virulence, especially in the nosocomial setting. We seek to understand synthesis, maintenance and remodeling of *S. aureus* cell wall to address lingering questions related to AMR mechanism beyond genetic level. We further study and engineer a specific class of hydrolases, PGHs, which eradicate multidrug-resistant *S. aureus* colonies on timescale spanning from few minutes to tens of minutes [2, 5].

References

[1] M. Karjalainen *et al.*, *J. Biomol. NMR* **74**, 741 (2020).

[2] L. Antenucci *et al.*, *eLife* **13**, rp93673 (2024).

[3] O. Aitio *et al.*, *Structure* **20**, 1692 (2012).

[4] H. Tossavainen *et al.*, *Manuscript in preparation*.

[5] V. Raulinaitis *et al.*, *Sci. Rep.* **7**, 6020 (2017).

Area-Selective Atomic/Molecular Layer Deposition of Photoluminescent Europium-Organic/Graphene Heterostructures

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Area-selective atomic-molecular layer deposition (AS-ALD/MLD) is a promising "bottom-up" alternative to the current nanopatterning techniques [1,2]. It has been used on a variety of materials, including the growth of two-dimensional materials (2DM). While there are examples of AS-ALD being used on 2DM, the approach of combining it with AS-MLD is still mostly unexplored. Due to the inherent 2D nature, the surface of 2DM does not provide sufficient reactive sites for chemisorption of ALD/MLD precursors compared with traditional microelectronics. Functionalization of certain surface areas is required to provide the selective growth of materials. Recently, we have overcome the chemical inertness of graphene to ALD precursors by local activation using direct femtosecond laser two-photon oxidation (TPO) [3] for selective ZnO deposition [4].

In this study, we guided the growth of Eu-organic (Eu-BDC) thin films on top of single-layer graphene via TPO (Figure 1). We achieved high homogeneity and more than 90% selectivity in locally activated predefined regions for Eu films up to 11 nm. The polymer used for graphene transfer significantly affects the selectivity of the ALD/MLD process, as it might leave residues and promote unnecessary deposition in pristine graphene areas. The fabricated graphene/Eu-organic thin films exhibited high photoluminescence at 612 nm even when excited with a 532 nm laser. The films are suitable for various applications in optoelectronics, sensors, and LEDs.

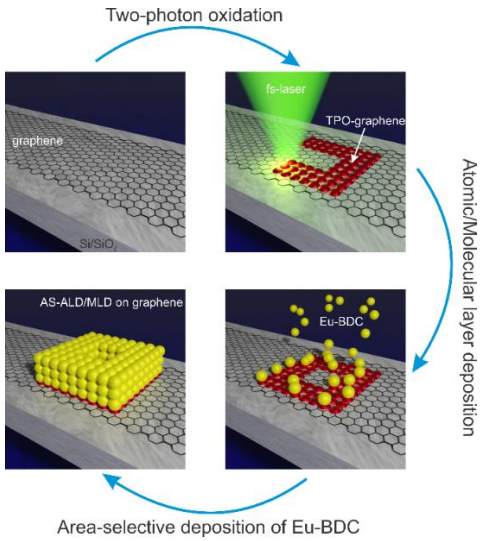

Figure 1: Scheme of the experiment, including TPO of graphene and ALD/MLD deposition of Eu-BDC thin films in predefined areas.

References

[1] G. N. Parsons, R. D. Clark, *Chem. Mater.* **32**, 4920 (2020).

[2] J. Multia, M. Karppinen, *Adv. Mater. Interfaces* **9**, 2200210 (2022).

[3] J. Aumanen, A. Johansson, J. Koivistoinen, P. Myllyperkiö, M. Pettersson, *Nanoscale* **7**, 2851 (2015).

[4] K. K. Mentel, A. V. Emelianov, A. Philip, A. Johansson, M. Karppinen, M. Pettersson, *Adv. Mater. Interfaces* **9**, 2201110 (2022).

The interplay between phage-bacteria-mucus on aged-Zebrafish

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The interaction between bacteriophages (phages) and mucus on metazoan surfaces has emerged as a critical area of research, with significant implications for both aquaculture and human health [1, 2, 3]. The bacteriophage adherence to mucus (BAM) model proposes a symbiotic relationship between metazoans and phages, where phages provide an external immunity against bacterial infections [1, 4]. This interaction is particularly relevant in aquatic environments, where fish are constantly exposed to potential pathogens [5]. Mucosal surfaces serve as a primary barrier against pathogens, with mucus playing a significant role in this defense [6, 7]. Mucin, primary component of mucus, influences the layer size of the mucosal matrix, regulating the diffusion of pathogens and other substances [6, 8, 9]. However, many factors could impact mucus production, and one example is the aging. Previous studies demonstrated that the physiological changes associated with aging affect mucus secretion and its protective roles, by increased mucous cell activity and variations in stress responses [10, 11, 12]. These age-related changes may further complicate phage-mucus interactions, highlighting the need for targeted research in this area. Fish, naturally covered by mucus layers [13], provide an excellent model for studying phage-mucus interactions and their implications for bacterial infections, particularly those affecting mucosal surfaces [1, 5, 7, 14]. Previous studies with Rainbow trout have shown that phages can bind to fish mucus, persisting for up to 7 days, and provide protection against bacterial pathogens such as *Flavobacterium columnare* [1]. However, the factors influencing phage binding to fish skin, particularly age-related changes in mucus production and composition, remain poorly understood. This research aims to elucidate the interplay between phages, bacteria, and mucus, in aged-zebrafish models. Zebrafish (*Danio rerio*) has emerged as an excellent model organism for studying host-pathogen interactions and mucosal immunity due to its transparency and well-characterized immune system [15, 16, 17]. By investigating how age affects phage binding to mucus, this research will gain valuable insights into the dynamics of mucosal immunity and bacterial infections. These findings could have far-reaching implications for developing novel strategies to combat bacterial infections in aquaculture and potentially in human health, addressing critical challenges in both fields.

References

[1] Almeida et al. Mbio. 10 (6) e-01984-19 (2019).
[2] Laanto et al. Front Microbiol. 6: 829 (2015).
[3] Chin et al. Proc Natl Acad Sci USA. 119 (27) e2116197119 (2022).
[4] Barr et al. Proc Natl Acad Sci USA. 110 (26) 10771-10776 (2013).
[5] Nakatani and Hori. Biology. 10 (2)166 (2021).
[6] Lieleg et al. Biophysical Journal. 98 (9)1782-1789 (2010).
[7] Bakshani et al. npj Biofil Microb. 4, 14 (2018).
[8] Fernández-Alacid et al. Sci of The Tot Envir. v. 644,1323-1335 (2018).
[9] Sanahuja et al. Front. Mar. Sci. 9 (2023).
[10] Sovran et al. Sci Rep. 9, 1437 (2019).
[11] Elderman et al. PLoS One. 12 (9): e0184274 (2017).
[12] Zheng et al. Front. Immunol. 13 (2022)
[13] Jakowska et al. Annals of The New York Acad Of Sci. 106 (2) 458-462 (1963).
[14] Jevtov et al. Sci Rep. 4, 6653 (2014).
[15] Celebi-Birand et al. Rec Adv Zebrafish Research. (2018).
[16] Cafora et al. Sci Rep. 9, 1527 (2019).
[17] Renshaw and Trede. Dis Model Mech. 5 (1): 38–47 (2012).

Electrochemical synthesis of nanomaterials for energy conversion and storage

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When designing an electroactive material, choosing the right chemical composition is a crucial but not the only task. The important aspect is maximizing the number of electroactive centers. It can be achieved by obtaining the chosen nanostructural material, providing a high surface-to-volume ratio. Nanostructurization can also be beneficial in the context of electrical conductivity, light trapping, etc. [1, 2].

In the presented research we developed different techniques for preparing nanostructural materials, mainly for application as electrode materials for electrochemical and photoelectrochemical water splitting. We chose cobalt selenide and iron selenide as an electrode material for electrochemical hydrogen evolution. We worked in two synthesis approaches: electrochemical-thermal, which was adapted for the preparation of thin cobalt selenide films on graphite, and direct – electrochemical which was applied to synthesize cobalt selenide films and nanowires and iron selenide films. Two-step synthesis consists of electrochemical cobalt deposition on graphite and its annealing in selenium vapors. We found that the composition of the obtained film can be controlled by process temperature. This technique allows us to obtain a thin crystalline film of cobalt diselenide. The direct electrochemical method consists of the electrodeposition of selenides from deep eutectic solvent (DES). We used a mixture called 'ethaline' (ethylene glycol and choline chloride in a 2:1 molar ratio 2:1) as a solvent for electrodeposition initiators. With this technique, we obtained amorphous cobalt selenide film deposited on graphite and crystalline iron selenide film on carbon paper.

As photoelectrodes for water splitting, we prepared nanowire arrays of tin oxide and copper oxide through template synthesis. Tin oxide nanowires were synthesized in a two-step method. Firstly, we electrodeposited the tin nanowires in a template that was annealed in the air in the second step. Obtained nanowires were composed mainly of tin dioxide. Copper oxide nanowires were prepared by constant potential electrodeposition into channels of AAO template, from a bath containing copper sulfate, lactic acid, alkalized with sodium hydroxide. Obtained nanowires were composed of cuprous oxide.

Prepared materials were characterized by scanning electron microscopy (SEM), and the composition was characterized by energy-dispersive X-ray spectroscopy (EDS), X-ray diffraction (XRD), and Raman spectroscopy. The electrocatalytic properties of cobalt selenide thin films were investigated in acidic media.

References

[1] Bhushan, Bharat, ed., *Springer handbook of nanotechnology*, *Springer*, (2017).
[2] Li, Jiangtian, and Nianqiang Wu, *Catal. Sci. Technol.* **5.3,** 1360-1384, (2015).

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Towards metasurfaces by DNA-assisted lithography

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In a past decade, DNA origami has become one of the most used building blocks in self-assembled materials in nanoscale [1]. Using DNA origami as tiles large 2D lattices have been assembled with different techniques [2]. In our recent work, we have demonstrated that within certain ionic conditions the blunt-ended Seeman Tile [3] origami forms ordered 2D lattices [4] on top of silicon, as shown in figure 2b. These can be further utilized in lithography processes, like in DNA assisted lithography (DALI) [5] shown in figure 1. Our final goal is to fabricate a layered metamaterial surface like the one in reference [6].

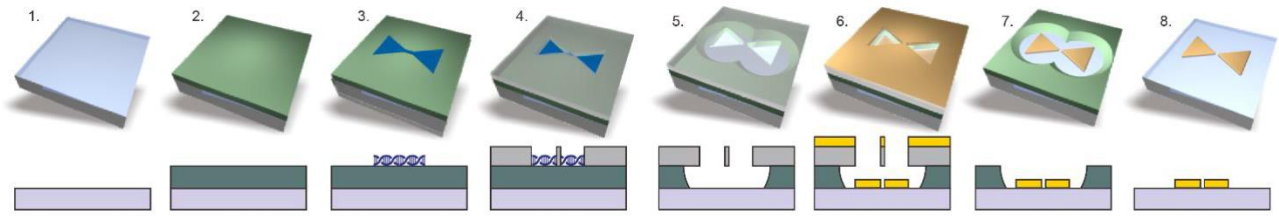

Fig. 1. DALI fabrication steps [5]: 1. Transparent substrate, 2. Silicon growth by Chemical Vapor Deposition, 3. Origami deposition, 4. SiO2 growth by the special CVD, 5. Isotropic Si etching by Reactive Ion Etching (RIE), 6. Au depositions by evaporation, 7. Lift-off by HF:HCl wet etching, 8. Removing of Silicon by RIE.

We have already successfully demonstrated the DALI up to step 5, *i.e.*, we have been able to grow silicon dioxide using the DNA lattice as a mask [5] shown in figure 2c. We have tried etching the silicon layer using the SiO_2 layer as a mask and imaged the results (figure 2d). We require a high precision etch process with large Si/SiO_2 selectivity and anisotropic etch profile (no undercut) to avoid the collapse of the silicon dioxide mask. We still need to optimize the etching process to get higher etching rate while keeping the profile (figure 2a). Therefore, the etch is done in cryogenic temperatures using SF_6 and O_2 as precursors. Using HBr instead of SF_6 is also a possibility and needs to more research with help of larger e-beam lithography structures and DNA lattice samples. HBr etching is done in higher temperatures. After etching is optimized, the next step is to use etched pattern as an evaporation mask to make the metallic nanostructures (step 6).

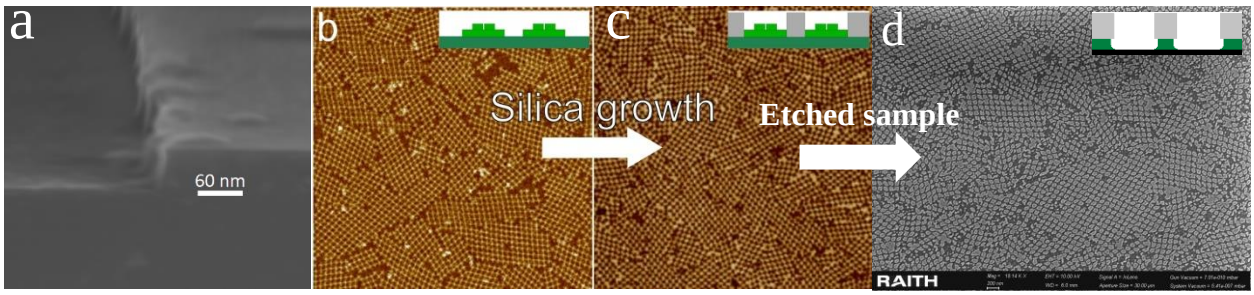

Fig. 2: a) SEM image for one e-beam lithography sample. b) AFM image of Seeman Tile fishnet-type lattice deposited on a silicon substrate. c) a Similar DNA lattice after silica growth, where origami shaped holes can be observed. d) SEM image of etched DNA lattice.

References

[1] F. Hong, F. Zhang, Y. Liu, et al., Chemical reviews 117, 12584-12640 (2017).
[2] J.M. Parikka, K. Sokołowska, N. Markešević, and J.J. Toppari, Molecules 26, 1502 (2021).
[3] W. Liu, et al., Angew. Chem. Int. Ed. 50, pp.264-267 (2011); A. Rafat, et al., Angew. Chem. Int. Ed. 53, 7665 – 7668 (2014).
[4] K. Tapio, C. Kielar, J.M. Parikka, A. Keller, H. Järvinen, K. Fahmy, and J.J. Toppari, Chem. Mat. 35, 1961–1971 (2023).
[5] B. Shen, V. Linko, K. Tapio, et al., Science advances 4, p.eaap8978 (2018).
[6] S. Xiao, U.K. Chettiar, A.V. Kildishev, V.P. Drachev, and V.M. Shalaev, Optics letters 34, pp.3478-3480 (2009).

Going beyond Sabatier's principle for a material descriptor and catalyst discovery in CO_2 to methanol thermoconversion

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Utilizing CO_2 into the production of useful chemicals, like methanol, closes the carbon loop and help with CO_2 emissions reduction. However, current catalysts for CO_2 hydrogenation suffer from low conversion rate, selectivity, and a lack of long-term stability. Experimental and theoretical search for new catalytic materials is expensive and time consuming. On the other hand, approximate methods, such as the Sabatier's principle, do not take into account the complexity of modern industrial catalysts consisting of polycrystals or nanoclusters with many facets and different sites [1].

In this work, we will present our novel descriptor – adsorption energy distribution – that we set to offer information for surfaces of miller indices in {-2,-1,0,1,2} and various adsorption sites. We considered four most important reactants and intermediates– H, OH, OCHO and OCH_3 (adsorbed radicals) [2] – for the distribution calculations. We follow with a workflow, employing highly efficient machine learning force-field from Open Catalyst project [3] and a validation procedure using density functional theory calculations of strategically selected datapoint. We apply this workflow for screening catalytic activity of single metals and bimetallic alloys. Finally, we will present our results for 159 materials, with over 800 000 calculations altogether, and classification of them using hierarchical clustering. The clustering links together materials like Cu-Zn, Pt-In and Ni-Zn alloys that are part of highly active catalysts [1], with new materials, which will be tested by our experimental collaborators.

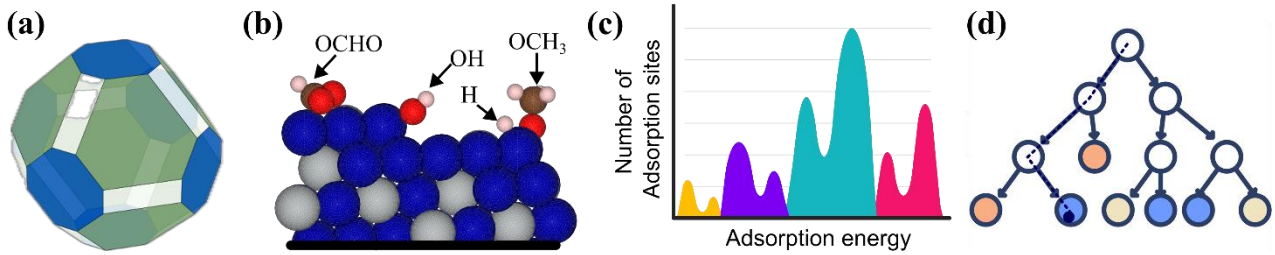

Figure 1: Industrial catalysts have multiple facets (a) and reactants and intermediates can occupy different binding sites (b). All of this is reflected in our novel descriptor called adsorption energy distribution (c) calculated with highly efficient machine learning force field. We employ unsupervised machine learning for clustering our results and prediction of materials catalytic activity (d).

References

[1] S. Bahri et al., *J. Clean. Prod.* **339**, 130653 (2022).

[2] P. Aman et al., *Science* **376**, 603 (2022).

[3] L. Chanussot et al., *ACS Catal.* **11**, 6059-6072 (2021); R. Tran et al., *ACS Catal.* **13**, 3066-3084 (2023); https://opencatalystproject.org/ .

CRISPR/Cas-Mediated Knockdown of PD-L1 and KRAS in Lung Cancer Cells

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Cancer cells can escape death and surveillance by the host immune system in various ways. Programmed cell death ligand 1 (PD-L1) is a transmembrane protein that is expressed by most cell types, including cancer cells, and can provide an inhibitory signal to its receptor PD-1, which is expressed on the surface of activated T cells, impairing the immune response. PD-L1/PD-1-mediated immune evasion is observed in several KRAS-mutated cancers. In the current study, we used the CRISPR/Cas9 system to knock down PD-L1 and KRAS in adenocarcinoma lung cells (A549 and H1975). Knockdown of PD-L1 was validated by qPCR and coculture with lymphocytes. The cells were functionally analyzed for cell cycle, migration and apoptosis. In addition, the effects of PD-L1 and KRAS downregulation on chemotherapy sensitivity and expression of inflammatory markers were investigated. Suppression of PD-L1 and KRAS led to a slowdown of the cell cycle in the G0/G1 phase and reduced migration, increased sensitivity to chemotherapy and triggered apoptosis of cancer cells. In addition, the conditioned medium of the modulated cells significantly affected the native cancer cells and reduced their viability and drug resistance. Our study suggests that dual silencing of PD-L1 and KRAS by CRISPR/Cas9 may be a promising therapeutic approach for the treatment of lung cancer [1].

References

[1] Abounar, S.A.; El-Nikhely, N.A.; Turkowski, K.; Savai, R.; Saeed, H. CRISPR/Cas-Mediated Knockdown of PD-L1 and KRAS in Lung Cancer Cells. Int. J. Mol. Sci. **25**, 9086 (2024).

Electrocatalytic Glucose Valorization Using Chiral Gold Nanorods

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Upgrading biomass is gaining considerable importance for establishing a clean and renewable chemical and energy infrastructure. Hydrogen production via water electrolysis is considered a green approach to sustainable fuel generation and renewable energy space [1]. However, the major challenge for scaling up to industrial level is the high energy consumption due to the thermodynamics and sluggish kinetics of the anodic oxygen evolution reaction (OER). Replacing the OER with alternative anodic reactions that require lower driving potential is a promising solution. Specifically, the oxidation of abundant, low-value carbohydrate biomass not only reduces the overall energy requirement but can also co-generate other valuable chemicals. Therefore, this co-electrolysis system also provides opportunities for industrial growth and recyclability of natural wastes.

Enantioselective catalysis using chiral nanomaterials has gained significant attention in recent years [2]. Achieving selective electrocatalytic transformations of complex organic compounds such as carbohydrates needs a fresh perspective to catalyst engineering. The adsorption of reactants and the selective cleavage of bonds to yield specific products strongly depend on the arrangement of active sites on the catalyst, i.e. surface structure. Using complex chiral ligands is the most common approach, but by developing chiral morphologies in inorganic nanomaterials, we can enable efficient electrocatalytic activity, high surface area, and novel reactivities.

In this work, we aim to study enantioselective glucose electrocatalysis using chiral Au nanorods with kinked structures. We prepared chiral gold nanorods by seed mediated wet chemical growth process and induced chirality using chiral amino acid to serve as the catalyst [3]. The properties of these Au nanorods were characterized by CD for degree of chirality, imaging via AFM, TEM and concentration analysis via UV. Glucose serves as a simple but relevant model representing the complex carbohydrates found in biomass. We expect that the unique kinked structures exposed on chiral Au nanorods could provide novel, selective electrocatalytic sites that could significantly improve the conversion efficiency of such biomass molecules [4].

References

1. Zhang, D.; Xu, Z.; Lee, J.; Ma, X.; Selective Electrocatalytic Hydrogenation of Lignocellulose-Derived 5-Hydroxymethylfurfural with Superior Productivities. *Appl. Catal. B* **2023**, *26* (10), 108003.
2. Chae, K.; Kim, J.; Lee, H.; The Promise of Chiral Electrocatalysis for Efficient and Sustainable Energy Conversion and Storage: A Comprehensive Review of the CISS Effect and Future Directions. *Chem. Soc. Rev.* **2024**, *53*, 1098–1112.
3. Ni, B.; Zhang, Y.; Wang, H.; Chiral Seeded Growth of Gold Nanorods Into Fourfold Twisted Nanoparticles with Plasmonic Optical Activity. *Adv. Mater.* **2023**, *35* (1), e2208299.
4. Zhu, Y. Q.; Jiang, C.; Wang, X.; Identification of Active Sites Formed on Cobalt Oxyhydroxide in Glucose Electrooxidation. *Angew. Chem., Int. Ed.* **2023**, *62* (15), e202219048.

The effect of photosensory module components on spectroscopic properties of a bacterial phytochrome

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Photoreceptor proteins, such as phytochromes, allow organisms to respond to changing light conditions. In optogenetics, these natural responses can be harnessed for human applications. To develop optogenetic tools, it is essential to fully understand the functional properties and the light-induced changes of these proteins. In previous studies, phytochromes have been extensively modified by mutating, truncating, and removing parts of the protein. In this work, we swapped the arm subdomain of the photosensory module from a bathy phytochrome to a canonical phytochrome of *Deinococcus radiodurans*. The arm has previously been proven to be a crucial component in signal transduction in phytochromes[1]. We employed UV-Vis, FTIR, and CD spectroscopy to study the photocycle of these phytochrome variants. Our results show that while photoconversion occurs, the stability of the illuminated state is altered in the arm-variants. Structurally, the arm appears to undergo rearrangement when converting from dark state to illuminated state. Furthermore, the environment around the chromophore is altered in the arm-variants. Here we show that the CD-signal of the chromophore in the illuminated state appears to differ between the arm-variants and the wild type protein. It remains uncertain whether these observations are due to faster reversion rates or impaired photoconversion. Deeper understanding about the photocycle will be captured by measuring the CD spectra of intermediate states by either cold trapping or applying time-resolved spectroscopy.

References

[1] M. Kurttila, J. Rumfeldt, H. Takala, and J.A. Ihalainen, *Structure.* **31**, 1100 (2023).

Poster 46

Selectively guiding excitation energy by collaborative light-matter coupling

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Strong light-matter coupling induces formation of polaritons, coherent superpositions of the excited states of the material and the confined light mode. In a typical Fabry-Pérot cavity strong coupling is achieved by introducing the coupled molecule inside the cavity in sufficient concentration. However, with the increased concentration the number of dark states, located at the molecular absorption energy, increases in proportion. Within all these hybrid states, i.e., the bright polaritons and the dark modes, the excitation is delocalized among all the molecules taking part in the coupling, and the excitation energy can easily be transferred from the bright polaritons to the dark states depending on their spectral overlap [1]. Simulations and experiments suggest that in their relaxation the polaritonic states, including the dark states, follow Kasha's rule and relax to the lowest energy state available for the system before decaying [1–4]. This hints that if a photoreactive molecule with the energy of the photoproduct well below the lower polariton is part of the superposition state, then the initially delocalized excitation will localize into one single reactive molecule which then undergoes the reaction bringing the system to its relaxed state [3].

Recently we have shown that the excitation spectrum of 10-hydroxybenzo[h]quinoline (HBQ) under strong coupling is a product of the excitation spectrum of the bare molecules and the absorption spectrum of the molecule-cavity system, suggesting that polaritons act as gateways for channeling an excitation into a molecule, which then proceeds normally and undergo excited state intermolecular proton transfer reaction like bare HBQ [5].

Here, we combine HBQ with an inert molecule with a strong absorption at the same energy, and form collaborative strong coupling of both molecules with the same cavity mode. In this case the excitation energy initially shared among all the molecules, is expected to rapidly localized into one of the reactive HBQ molecules. By varying the amounts and ratio between the molecules we investigate the efficiency of the excitation energy guiding. The phenomenon could be utilized for example in the enhanced light-harvesting [3].

References

[1] H.L. Luk, J. Feist, J.J. Toppari, G. Groenhof, J. Chem. Theory Comput. 13, 43244335 (2017).

[2] S. Baieva, O. Hakamaa, G. Groenhof, T.T. Heikkila, J.J. Toppari, ACS Phot. 4, 2837 (2017).

[3] G. Groenhof, J.J. Toppari, J. Phys. Chem. Lett. 9, 4848 (2018).

[4] E. Hulkko, S. Pikker, V. Tiainen, R.H. Tichauer, G. Groenhof, J.J. Toppari, J. Chem. Phys. 154, 154303 (2021).

[5] Dutta, A., Tiainen, V., Sokolovskii, I. et al. Nat Commun 15, 6600 (2024).

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