Nanoscience Days 2025

Abstract book

NSC
FINLAND

Jyväskylä, Finland

October 7-8, 2025

Plenary Speakers

1. Laura Na Liu – *Programmable DNA Architectures: From Reconfigurable Synthetic Cells to Moiré Superlattices*
2. Qi Chen – *Understanding the "sperm RNA code" for epigenetic inheritance with emerging tools*
3. Mariana Rossi (online) – *TBA*
4. Menno Veldhorst – *TBA*
5. Giuseppe Balistreri – *Development of efficient antivirals and non-invasive imaging of virus infection in the brain*
6. Sijbren Otto – *Steps in building a minimal form of life*
7. Simone Taioli – *Predict, Probe, Reconstruct — Electron Correlation Across Scales: Beams, Bands, and Galactic Chemical Evolution*
8. Jose Baldovi – *Tunable Magnetism in 2D Materials: A Playground for Solid-State Physics*
9. Peter Hegeman – *TBA*

Plenary 1: Laura Na Liu

Plenary 2: Qi Chen

Understanding the ‘sperm RNA code’ for epigenetic inheritance with emerging tools

Qi Chen

University of Utah School of Medicine, Salt Lake City, Utah, USA
Website: http://qichen-lab.info/

Abstract:
Recent discoveries have revealed a novel layer of inheritance, showing that mammalian sperm transmit not only DNA but also diverse RNA molecules that mediate the intergenerational effects of environmental exposures (e.g., diet, stress, toxins). Expanding knowledge of sperm RNAs—including miRNAs, tsRNAs, rsRNAs, and lncRNAs—together with their modifications and spatial compartmentalization, supports the emerging concept of a ‘sperm RNA code’ that programs offspring phenotypes during development. I will discuss the challenges and opportunities in establishing this field, including identifying the key sperm RNAs responsible for paternal phenotype transmission, uncovering their native expression and modification profiles with advanced sequencing tools, and understanding the molecular events they trigger in embryos. Complete deciphering of the sperm RNA code under different environmental conditions could transform our understanding of epigenetic inheritance and open paths toward translational applications and precision medicine.

Plenary 3: Mariana Rossi (online)

Plenary 4: Menno Veldhorst

Plenary 5: Giuseppe Balistreri

Plenary 6: Sijbren Otto

Steps in Building a Minimal Form of Life

Sijbren Otto
Centre for Systems Chemistry, Stratingh Institute, University of Groningen, Nijenborgh 3, 9747 AG Groningen, the Netherlands; s.otto@rug.nl https://www.otto-lab.com/

Abstract: How the immense complexity of living organisms has arisen is one of the most intriguing questions in contemporary science. We have started to explore experimentally how organization and function can emerge from complex molecular networks in aqueous solution.[1] We focus on networks of molecules that can interconvert, to give mixtures that can change their composition in response to external or internal stimuli (Figure 1). Noncovalent interactions *within* molecules in such mixtures can lead to the spontaneous formation of foldamers of remarkable structural complexity.[2,3] In contrast, molecular recognition *between* molecules in such mixtures leads to their mutual stabilization, which drives the synthesis of more of the privileged structures. As the assembly process drives the synthesis of the very molecules that assemble, the resulting materials can be considered to be self-synthesizing. In this process the assembling molecules are replicating themselves, where replication is driven by self-recognition of these molecules in the dynamic network.[4] We have witnessed spontaneous differentiation (a process akin to speciation as it occurs in biology) in a system made from a mixture of two building blocks.[5] When such systems are operated under out-of-equilibrium conditions, replicators can complexify.[6]

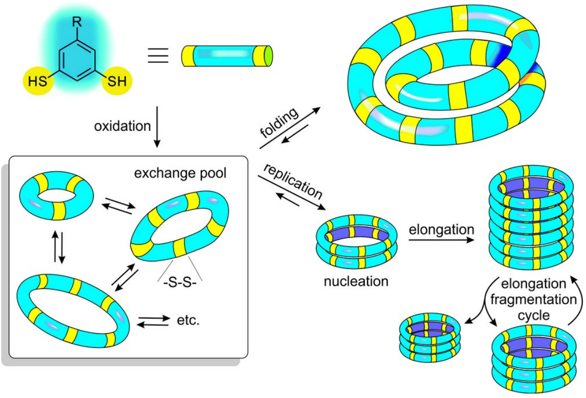


Figure 1. *Molecular recognition within molecules yields foldamers and between molecules drives self-replication.*

Replicators that are able to catalyse reactions other than their own formation have also been obtained, representing a first step towards metabolism.[7,8] Rudimentary Darwinian evolution of purely synthetic molecules has also been achieved [9,10] and the prospect of synthesizing life de-novo is becoming increasingly realistic.[11,12]

1. Li, J.; Nowak, P.; Otto, S. *J. Am. Chem. Soc.* **2013**, 135, 25, 9222-9239.
2. Liu, B.; Pappas, C. G.; Zangrando, E.; Demitri, N.; Chmielewski, P. J.; Otto, S. *J. Am. Chem. Soc.* **2019**, *141*, 1685-1689.
3. Pappas, C. G.; Mandal, P. K. Liu, B.; Kauffmann, B.; Miao,X.; Komáromy, D.; Hoffmann, W.; Manz, C.; Chang, R.; Liu, K.; Pagel, K.; Huc, I.; Otto, S. *Nature Chem.* **2020**, *12*, 1180–1186.
4. Carnall, J. M. A.; Waudby, C. A.; Belenguer, A. M.; Stuart, M. C. A.; Peyralans, J. J.-P.; Otto, S. *Science* **2010**, *327*, 1502-1506.
5. Sadownik, J. W.; Mattia, E.; Nowak, P.; Otto, S. *Nature Chem.* **2016**, *8*, 264–269.
6. Yang, S.; Schaeffer, G.; Mattia, E.; Markovitch, O.; Liu, K.; Hussain, A. S.; Ottelé, J.; Sood, A.; Otto, S. *Angew. Chem. Int. Ed.* **2021**, *60*, 11344-11349.
7. Monreal Santiago, G.; Liu, K.; Browne, W. R.; Otto, S. *Nature Chem.* **2020**, *12*, 603-607.
8. Ottelé, J.; Hussain, A. S.; Mayer, C.; Otto, S. *Nature Catal.* **2020**, *3*, 547-553.
9. K. Liu, A. Blokhuis, C. van Ewijk, A. Kiani, J. Wu, .W.H. Roos, S. Otto *Nature Chem.* **2024**, *16*, 79–88.
10. Eleveld, M.; Geiger, Y.; Wu, J.; Kiani, A.; Schaeffer, G.; Otto, S. *Nature Chem.* **2025**, *17*, 132-140.
11. Adamski, P.; Eleveld, M.; Sood, A,; Kun, A.; Szilágyi, A.; Czárán, T.; Szathmáry, E.; Otto, S. *Nature Rev. Chem.* **2020**, *4*, 386–403.
12. Otto, S. *Acc. Chem. Res.* **2022**, *55*, 145-155.

Plenary 7: Simone Taioli

Predict, Probe, Reconstruct — Electron Correlation Across Scales: Beams, Bands, and Galactic Chemical Evolution

In this presentation, we introduce a general theoretical and computational framework that combines ab initio and Monte Carlo methods to study the electronic, optical, mechanical and transport properties of materials across different time and length scales [1,2].

Photon, electron and ion beams are used as probes to perturb the target system. This allows us to obtain information about the excitation spectrum and compare the results directly with experimental data. Our approach models elastic and inelastic collisions of the impinging particles using first-principles simulations: We solve the Dirac-Hartree-Fock equations and calculate the macroscopic dielectric response function either using high-precision linear-response time-dependent density functional theory or from experimental optical spectra.

Inelastic scattering channels include single-particle and collective (plasmon) excitations, polaron and electron-phonon interactions, ionisation and Auger emission, all of which contribute to energy loss and momentum transfer to the medium. Our model also takes into account the generation of secondary electrons during the ionisation of atoms. The resulting elastic and inelastic scattering cross sections are fed into a Monte Carlo routine enabling the simulation of electron cascade trajectories.

The excellent agreement of our simulations with experimental Auger electron spectra (AES), reflection electron energy-loss spectra (REELS), secondary electron (SE) spectra, and total electron yield (TEY) across metals, insulators, semiconductors, and biologically relevant materials demonstrates the robustness and versatility of our framework.

We will illustrate a broad range of applications, including:

- charging of test masses by cosmic radiation for the upcoming mission of the Laser Interferometer Gravitational Wave Observatory (LISA) [3];
- material growth [4];
- dose deposition and DNA damage in hadron therapy for cancer treatment [5];
- advanced imaging techniques, including atom probe tomography with single-cycle terahertz laser pulses [6];
- beta-decay of isotopes in astrophysical scenarios relevant for nucleosynthesis of heavy elements in stars [7].

1) Electron spectroscopies and inelastic processes in nanoclusters and solids: Theory and experiment, S Taioli, S Simonucci, L Calliari, M Dapor, *Physics reports* 493 (5), 237-319 (2010)

2) Advancements in Secondary and Backscattered Electron Energy Spectra and Yields Analysis: from Theory to Applications, S Taioli, M Dapor, *Surface Science Reports* 80, 100646 (2025)

3) The role of low-energy electrons in the charging process of LISA test masses, S Taioli, M Dapor, F Dimiccoli, M Fabi, V Ferroni, C Grimani, M Villani, W J Weber, *Classical and Quantum Gravity* 40, 075001 (2023)

4) Epitaxy of nanocrystalline silicon carbide on Si (111) at room temperature, R Verucchi et al., *Journal of the American Chemical Society* 134 (42), 17400-17403 (2012)

5) Relative Role of Physical Mechanisms on Complex Biodamage Induced by Carbon Irradiation, S Taioli, PE Trevisanutto, P de Vera, S Simonucci, I Abril, R Garcia-Molina, M Dapor, *The Journal of Physical Chemistry Letters* 12 (1), 487-493 (2020)

6) Evaporation of cations from non-conductive nano-samples using single-cycle THz pulses: an experimental and theoretical study, M De Tullio et al. *Physical Review B* 111 (4), 045428 (2025)

7) Theoretical estimate of the half-life for the radioactive ^{134}Cs and ^{135}Cs in astrophysical scenarios, S Taioli et al., *The Astrophysical Journal* 933, 158 (2022)

Plenary 8: Jose Baldovi

Plenary 9: Peter Hegeman

Poster Presentations

1. Mohammad Bagheri – *Lateral Graphene-Metallene Interfaces at the Nanoscale*
2. Leo Bellassai – *Photon-assisted stochastic resonance in nanojunctions*
3. Marko Melander – *Recent advances in atomistic theory and simulation of electrochemical systems*
4. Dimitri Delcourt – *Programmable assembly of double and triple helix in water*
5. Nima Nematimansur – *Toward spin-photon interfaces*
6. Meeri Niemi – *Characterisation of a novel jumbophage collection*
7. Karyna Karneyeva – *FKy-1 Phage: The First Model for Deciphering Megaphage Biology*
8. Jaismon Francis – *Resolving Anisotropy and Impurities: A Hybrid DLS-Microscopy Approach for Characterizing MWNT Dispersions*
9. Niina Harju – *Hydroquinone disrupts mitochondria and protein levels*
10. Brenda de Souza Ferrari – *Machine Learning-Assisted Clustering of Amino Acids: The Development of an Interaction Model of the Protein-Nanocluster Interface*
11. Louise Miton – *Harnessing Multi-Stranded Helices for Molecular Links, Knots and Topological Hydrogels*
12. Vilma Tarkiainen – *Mammalian optogenetic tool utilizing bacteriophytochrome-based two-component signaling*
13. Julia Naulapää – *Cloud point extraction of pyridine N-oxides using water-soluble calix[4]pyrroles*
14. Hanna Jääskö – *Electronic and Optical Properties of Metal-Ion-Mediated Au25 Nanocluster-Based Assemblies*
15. Henna Rahkola – *Solvent-induced gelation: Effect of terminal functionality*
16. Arpan Dutta – *Organic excitonic nanostructures for weak and strong coupling*
17. Yomi Matsumoto-Viljanen – *Antibacterial and antiviral properties of Finnish berries*
18. Thiwangi Nimesha Rajapaksha Rajapaksha Pathirannehelage – *Increasing the domain size of DNA origami lattices on silicon*
19. Pedro Portugal – *Floquet-engineering heat pulses in one-dimensional wires*
20. Maryam Darvishi – *Josephson effect at arbitrary disorder strength in systems with generic spin-dependent fields*
21. Virginia Ranaweera – *PDMS as a flexible substrate for graphene biosensors*
22. Oscar Moreno Segura – *Bias-Driven Electroluminescence in Molecular Junctions*

23. Joona Marjamäki – *Nonequilibrium dynamics in the spin-boson model*
24. Aku Lempelto – *A computational exploration of photocatalytic hydrogen and oxygen evolution reaction pathways in low-dimensional Ni/MoS2 systems*
25. Maryam Naderpour – *Area-selective ALD as dielectric for top-gated GFET*
26. Eeki Tarkkonen – *Anion-modulated iminium catalysts*
27. Zhuoran Geng – *Phonon-Blocked Junction Calorimeter*
28. Pooja Sudha – *A mechanical device engineered for coherent control of spin*
29. Aino Rolig – *Towards total synthesis of humilisin E: Finding strategies for construction of the 9-membered ring*
30. Işılay Öztürk – *Investigation of Au22KCK16 Nanocluster and Reactive Oxygen Species (ROS)*
31. Arash Mousavi Cheghabouri – *Compact Mach–Zehnder Interferometer Design for Improved Optomechanical Measurements in a Cryogenic Environment*
32. Toivo Hakanen – *NbTiN-based superconducting refridgerators*
33. Aki Ruhtinas – *Fabrication of quantum devices with focused helium ion beam*
34. Milla Männikkö – *Silicon optomechanical devices for spin coupling*
35. Roosa Vanhatalo – *Temperature-controlled intermediates in the photocycle of the phytochrome from Deinococcus radiodurans*
36. Pradip Kumar Mondal – *ECH catalyzed Enantioselective Hydration of 2E-Enoyl-SPAN via Simultaneous Activation of the Active Site Oxyanion Hole and Activation of H2O molecule.*
37. Andrii Chepurnyi – *Neural network acceleration of numerical simulation of methane combustion in a gas turbine engine*
38. Bharat Chand Bathu – *Visualising Kondo lattice behaviour in the air-stable ferromagnet Ta3FeS6*
39. Ville Tiainen – *Beyond Polariton Filtering: New Pathways for Polariton-Mediated Excitation*
40. Natale Matranga – *Beyond Eliashberg Theory of Superconductivity in flat-band systems*
41. Ilona Rissanen – *Structural biology of infection and immunity*
42. Eetu Hakkarainen – *Controlling Phosphorescence of Bisphosphonium Salts*
43. Markus Ahlskog – *The water droplet contact line probed with multiwalled carbon nanotubes at the air-water interface*
44. Kasperi Paloniemi – *A new technique based on multiwalled carbon nanotubes for exploring early phase spreading of water droplets*

Poster 1

Lateral Graphene-Metallene Interfaces at the Nanoscale

Mohammad Bagheri[1], Pekka Koskinen[1]
[1]*Nanoscience Center, Department of Physics, University of Jyväskylä, 40014 Jyväskylä, Finland*
Contact: mohammad.m.bagheri@jyu.fi

Metallenes are atomically thin, nonlayered two-dimensional materials [1-2]. While they have appealing properties, their isotropic metallic bonding makes their stabilization difficult and presents considerable challenges to their synthesis and practical applications [3-5]. However, their stabilization can still be achieved by suspending them in the pores of two-dimensional template materials, making the properties of lateral interfaces of metallenes scientifically relevant. Here, we combined density-functional theory and universal machine-learning interatomic potentials to study lateral interfaces between graphene and 45 metallenes with various profiles. We optimized the interfaces and analyzed their energies, electronic structures, and stabilities against temperature effects, defect formation, and structural deformations. We found that the interfaces are the most stable energetically and with respect to lattice mismatch, defect formation, and lateral strain when their profiles were geometrically smooth. The most stable interfaces are found for transition metals. In addition, we demonstrate how universal machine-learning interatomic potentials now offer the accuracy required for the modeling of graphene-metallene interfaces. By systematically expanding the understanding of metallenes' interface properties, we hope these results guide and accelerate their synthesis to enable future applications and benefit from metallenes' appealing properties [6].

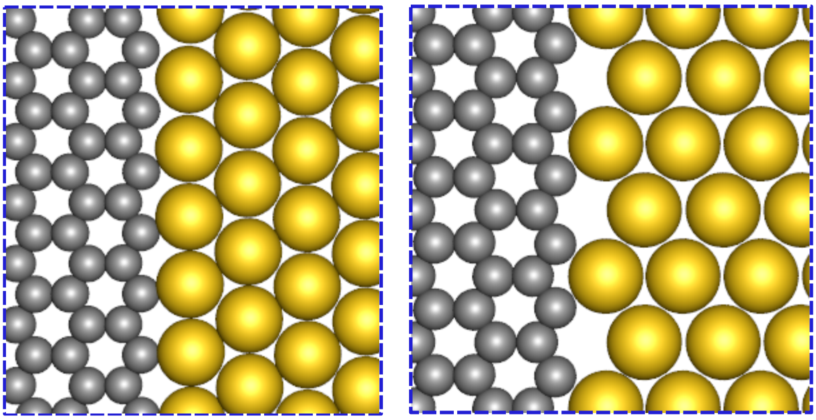


Figure 1: Schematic atomic structures of lateral graphene/metallene interfaces.

References

[1] J. Nevalaita & P. Koskinen *Phys. Rev. B* **97** (2018).

[2] J. Nevalaita & P. Koskinen *Phys. Rev. B* **98** (2018).

[3] J. Nevalaita & P. Koskinen *Nanoscale* **11** (2019).

[4] K. R. Abidi & P. Koskinen *Nanoscale* **16** (2024).

[5] K. R. Abidi, M. Bagheri, S. Singh & P. Koskinen *2D Mater.* **12** (2025).

[6] M. Bagheri & P. Koskinen, Lateral interfaces of graphene-metallenes at nanoscale *(under review)* (2025).

Poster 2

Photon-assisted stochastic resonance in nanojunctions

Michael Ridley[1], Leo Bellassai[2], Michael Moskalets[3,4],Lev Kantorovich[5],Riku Tuovinen[2]
[1]*Faculty of Engineering and Institute of Nanotechnology and Advanced Materials, Bar Ilan University, Ramat Gan 52900, Israel*
[2]*Department of Physics, Nanoscience Center, P.O. Box 35, 40014 University of Jyväskylä, Finland*
[3]*Institute for Cross-Disciplinary Physics and Complex Systems IFISC (UIB-CSIC), 07122 Palma de Mallorca, Spain*
[4]*Department of Metal and Semiconductor Physics, NTU "Kharkiv Polytechnic Institute",*
61002 Kharkiv, Ukraine
[5]*Theory and Simulation of Condensed Matter (TSCM), King's College London, Strand, London WC2R 2LS, United Kingdom*
Contact: lebellas@jyu.fi

We study stochastic resonance in molecular junctions driven by a periodically-varying external field. This is done using the time-dependent Landauer-Büttiker formalism, which follows from exact analytical solutions to the Kadanoff-Baym equations describing the molecular junction subject to an arbitrary time-dependent bias. We focus on a double quantum dot nanojunction and compare the effects of the temperature with the fluctuating bias in the statically-driven case. We then consider the combined effect of AC-driving and white noise fluctuations on the rectified current through the nanojunction, and find a stochastic resonance effect, where at certain driving conditions the bias fluctuations enhance the current signal. The study is then extended to include the color noise in the applied bias, so that the combined effect of the color noise correlation time and driving frequency on stochastic resonance is investigated. We thereby demonstrate that photon-assisted transport can be optimized by a suitably tuned environment.

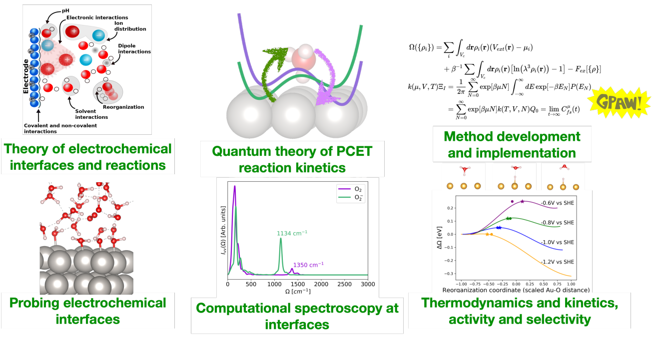
Poster 3

Recent advances in atomistic theory and simulation of electrochemical systems

Marko M. Melander[1]
[1] *Department of Chemistry, Nanoscience Center, University of Jyväskylä, Finland*
Contact: marko.m.melander@jyu.fi

Electrochemistry enables the efficient interconversion of electric and chemical energy which can be harnessed in numerous electrocatalytic reactions such as hydrogen evolution and oxidation, oxygen reduction, and CO_2 reduction reactions. At the heart of all electrochemical and electrocatalytic systems lies the ability to control reaction thermodynamics and kinetics at solid-liquid interfaces through the application of an external electrode potential. While experiments are readily performed under such conditions, theory and simulation of electrochemistry under conditions mimicking experiments is extremely difficult requiring the development and application of novel theoretical and modelling methods.

In my contribution, I will present our recently developed theoretical and computational methods for simulating electrocatalytic thermodynamics[1,2] and kinetics[3] under constant potential conditions within the grand canonical ensemble (GCE) approach. I will also present ways to simulate the electrolyte effects on electrochemical interfaces and reactions. Illustrative applications these methods showcase 1) the complex surface chemistry of gold electrodes as a function of potential and pH [4], 2) the simulation of interfacial thermodynamics [5], 3) the effect cations on the CO_2 reduction reaction mechanism, thermodynamics, and kinetics [6], and 4) the effect of the electrode potential in creating localized electronic (polaron) states for activating semiconductor interfaces towards the hydrogen evolution reaction[7]. Overall, I will present how advanced theory and computational methods can be used to understand the impact of the catalyst and reaction conditions in electrocatalysis from the atomic level.



References

[1] M.M. Melander, M.J. Kuisma. T.E.K. Christensen, K. Honkala, J. Chem. Phys. 150, 041706 (2019)
[2] M.M. Melander, T. Wu, T. Weckman, K. Honkala, *npj Computational Materials volume 10, 5 (2024)*
[3] M.M. Melander, J. Electrochem. Soc., 167, 116518 (2020)
[4] K. Moradi, M.M. Melander, *submitted*, DOI: 10.26434/chemrxiv-2025-13r9v-v2
[5] F. Domínguez-Flores, T. Kiljunen, A. Groß, S. Sakong, M.M. Melander, J. Chem. Phys. 161, 044705 (2024)
[6] X. Qin, H.A. Hansen, K. Honkala, M.M. Melander, Nature Communications volume 14, 7607 (2023)
[7] T. Wu et al, *submitted,* DOI: 10.26434/chemrxiv-2024-j7thd-v2

This work was supported by The Academy of Finland through grants 307853, 338228, and 317739

Poster 4

Programmable assembly of double and triple helix in water

Dimitri Delcourt[1], Reguram Arumugaperumal[1], Prachi Verma[1], Perttu Permi[1], Antonio Frontera[2], Fabien B. L. Cougnon[1]
[1] *Nanoscience Center and Chemistry Department, University of Jyväskylä, Finland*
[2] *Department de Química, Universitat de les Illes Balears, 07122 Palma de Mallorca, Baleares, Spain*
Contact: dimitri.j.delcourt@jyu.fi

In nature, biomolecules adopt different types of helical structures that alter their properties and functions [1]. Single-, double- and triple helices are observed in enzymes, DNA and collagen respectively [2]. By mimicking nature, chemists have worked on the helical self-assembly of purely artificial strands; the ability of *m*-oligophenylene ethynylene to fold into single helices is well documented [3]. The selective assembly of higher order helices requires sophisticated strands to be designed and synthesized. Here we propose a simple system in which the strands are programmed to access double- or triple helices in water. The strands have been designed in such a way that their sequences of hydrophobic and hydrophilic fragments promote the folding via solvophobic, π-stacking and electrostatic interactions. These helices possess a hydrophobic cavity capable to host sulfonate or other negatively charged guests. From simple components, we build complex supramolecular assemblies suitable for the catalysis of amphiphilic molecules.

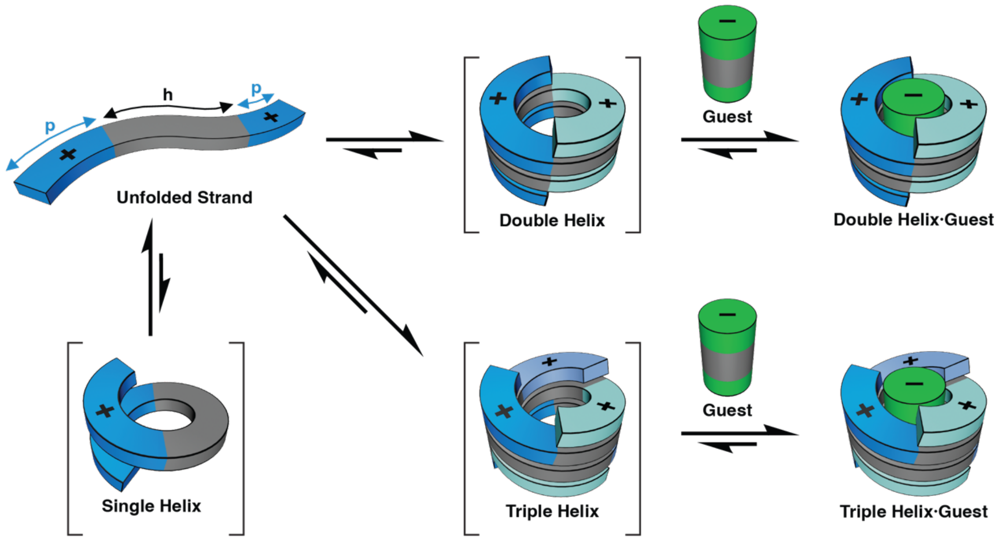


Figure 1. Schematic representation of the positively charged strand folding into helices in water in the presence of a negatively charged guest.

Figure 1: Schematic representation of the positively charged strand folding into helices in water in the presence of a negatively charged guest.

References

[1] (a) *Nano Lett.*, **20**, 8, 5597–5600 (2020); (b) *Chem. Soc. Rev.*, Advance Article (2022).
[2] (a) *Nature*, **171**, 737-738 (1953); (b) *Org. Biomol. Chem.*, **17**, 8031-8047 (2019).
[3] (a) *Chem. Rev.*, **101**, 3893-4012 (2001); (b) *Chem. Rev.*, **116**, 13752- 13990 (2016).
[4] BindFit v0.5.
[5] EXSYCalc.

Poster 5

Toward spin-photon interfaces

Nima Nematimansur[1], Juha Muhonen[1]
[1]Department of physics, University of Jyväskylä,
Contact: nima.n.nematimansur@jyu.fi

One of the most promising candidates for harnessing the power of quantum information processing is to use the benefits of spins and photons in a single hybrid platform. The coupling of spins and photons unites the computational strength of spin qubits with the communication efficiency of photons[1]. Here, we study photon sources in silicon—a highly studied, developed, and mature material—and we aim to characterize the photon emission characteristics from transitions involving spins, and eventually integrate them with silicon photonics and spin control measurements.

In this stage of our work, we assemble an optical spectroscopy setup optimized for optical readout of the photons radiated from bound exciton recombination.

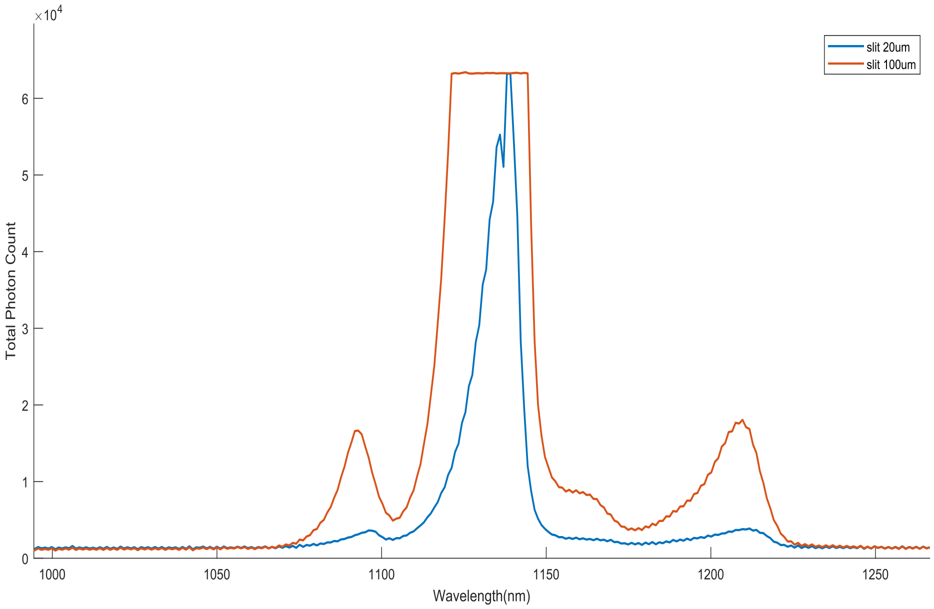


Figure 1: *Photoluminescence of P-doped silicon mounted in a continuous-flow liquid He cryostat*

References

[1] C. C. Lo, et al. , “Hybrid optical-electrical detection of donor electron spins with bound excitons in silicon”, Nature Materials 14, 2015

Poster 6

Characterisation of a novel jumbophage collection

Meeri Niemi[1], Karyna Karneyeva[1], Hanna M. Oksanen[2], Elina Laanto[1]
[1]Department of Biological and Environmental Science, Faculty of Mathematics and Science, University of Jyväskylä, Finland
[2]Molecular and Integrative Biosciences Research Programme, Faculty of Biological and Environmental Sciences, University of Helsinki, Finland
Contact: meeri.fm.niemi@jyu.fi

Despite the abundance of bacteriophages (phages) in nature, their true diversity remains largely unexplored, particularly for large phages known as jumbophages, which have genomes exceeding 200 kb [1]. We isolated a collection of 39 phages from boreal freshwater environments, 8 of which were classified as jumbophages. This finding suggests that jumbophages may be highly abundant in these ecosystems. To explore potential shared traits among jumbophages, we 1) characterised genomes using whole genome sequencing, 2) examined virion morphology with electron microscopy, and 3) investigated the presence of a "phage nucleus" structure using fluorescence microscopy. Our analyses revealed that the jumbophage genomes clustered into three length categories: approximately 230 kb, 320 kb and 380 kb. Genomic comparisons showed that these phages mostly exhibit minimal similarity to one another, highlighting the remarkable genetic diversity among large phages. These genomes encode diverse features, with an unprecedented number of tRNA genes, up to 63 in a single phage genome, alongside various anti-defence systems. The jumbophages displayed a typical tailed virion morphology, with large capsids reaching up to 150 nm in diameter. Notably, we observed a single instance of phage nucleus formation in a phage infecting Pseudomonas sp. These findings advance our understanding of the largely unexplored diversity and unique features of jumbophages, highlighting traits that may potentially reveal novel insights into viral evolution and ecological roles.

References

[1] Al-Shayeb, B., et al. *Nature* **578**, 425–431 (2020).

Poster 7

FKy-1 Phage: The First Model for Deciphering Megaphage Biology

Karyna Karneyeva[1], Sebastian Kokko[2], Emmanuelle Neumann[3], Guy Schoehn[3], Hanna M. Oksanen[2], Elina Laanto[1]
[1]*Department of Biological and Environmental Science, Faculty of Mathematics and Science, University of Jyväskylä, Survontie, 40500, Jyväskylä, Finland*
[2]*Molecular and Integrative Biosciences Research Programme, Faculty of Biological and Environmental Sciences, University of Helsinki, Viikinkaari, 00790, Helsinki, Finland*
[3]*Institute for Structural Biology, Université Grenoble Alpes, Av. Centrale, 38400, Grenoble, France*
Contact: karyna.a.karneyeva@jyu.fi

The discovery of megaphages has extended the known size limits of bacteriophages far beyond expectations. Their enormous genome sizes, exceeding 600 kbp, seem counterintuitive for a host-dependent lifestyle. This raises fundamental questions: are megaphages evolutionary outliers, or does a large genome provide adaptive advantages?

Megaphages were initially discovered through sequence data [1]. In silico methods reveal valuable insights into viral diversity, yet megaphage biology remains largely unexplored due to the lack of isolates. So far, it has been assumed that the main limitation of in vivo research is the inefficacy of standard phage isolation methods, along with the challenges of cultivating putative hosts.

In our laboratory, we study unique megaphages from boreal freshwater ecosystems that infect *Flavobacterium* strains. The first isolated representative is the FKy-1 phage. Morphologically, it is a myovirus with an ~160 nm icosahedral head and a ~180 nm tail. Its genome spans 646,765 bp and encodes 1,068 CDSs, 64 tRNA genes, 6 tmRNAs, and diverse auxiliary metabolic genes. Comparative analyses place FKy-1 within the Mahaphage clade — the largest of the 10 phylogenetic groups of huge phages from diverse ecosystems [2] — rather than with smaller phages infecting the *Flavobacteriaceae* family. Still, FKy-1 shares no more than 34% nucleotide-based intergenomic similarity with megaphage representatives from metagenomic datasets.

Our data show that the progeny yield of FKy-1 is lower than that of smaller-genome phages. This raises key evolutionary questions about the competitive capabilities of megaphages. Our specific interest lies in the co-infection of bacterial hosts by megaphages and smaller phages. We are investigating whether megaphages gain advantages, such as faster host takeover, and how competition unfolds within bacterial cultures.

Taken together, we propose FKy-1 as a valuable model for exploring the unique biology of megaphages.

References

[1] Devoto, A.E. et al. Nat Microbiol 4, 693-700 (2019).

[2] Al-Shayeb, B. et al. Nature 578, 425-431 (2020).

Poster 8

Resolving Anisotropy and Impurities: A Hybrid DLS-Microscopy Approach for Characterizing MWNT Dispersions

Jaismon Francis[1], Paloniemi Kasperi[1], Markus Ahlskog [1]
[1] Department of Physics and Nanoscience Center, University of Jyväskylä, Survontie 9, 40014, Jyväskylä, Finland
Contact: markus.e.ahlskog@jyu.fi

The downstream performance of materials incorporating multi-walled carbon nanotubes (MWNTs) depends on the nanotube dimensions and dispersion state, but their quantitative in situ characterisation remains a significant challenge. While direct imaging techniques such as electron microscopy are powerful, they are ex situ, statistically limited, and require sample preparation that can alter the native state of aggregation. Conversely, Dynamic Light Scattering (DLS) is a rapid and statistically robust method for size analysis [1]. However, DLS data interpretation presents a significant challenge for high-aspect-ratio, optically anisotropic nanoparticles, particularly in non-aqueous media.

This work establishes a systematic protocol for preparing and characterizing kinetically stable MWNT dispersions in 1,2-dichloroethane. Through rigorous optimization of sonication energy and concentration, we achieve dispersions exhibiting a primary hydrodynamic diameter of approximately 240 nm. This apparent size, however, convolutes the nanotubes' physical dimensions with contributions from impurities, such as co-existing amorphous carbon, and the complex hydrodynamics of nanotubes.

Our forward-looking aims are therefore threefold: (1) To employ time-resolved DLS to quantify the aggregation kinetics and long-term stability of the dispersed phase [2]. (2) To utilize Multi-Angle DLS (MADLS) to deconvolve the population distributions of MWNT bundles and amorphous carbon impurities. (3) To implement a Depolarized DLS (DDLS) analysis, accounting for both translational and rotational diffusion, to extract the true physical length and diameter of the nanotubes [1]. Ultimately, this work seeks to develop a rigorous hybrid methodology, correlating DLS-derived parameters with direct imaging techniques, to provide a critical tool for the quality control and rational design of high-performance nanotube-based systems.

References

[1] Badaire, Stéphane, et al. Langmuir **20**, 24 (2004).

[2] Ju, Li, et al. Colloids and Surfaces A: Physicochemical and Engineering Aspects **409** (2012).

Poster 9

Hydroquinone disrupts mitochondria and protein levels

Niina Harju[1]
[1]*School of Pharmacy, University of Eastern Finland, Yliopistonranta 8, 70210 Kuopio, Finland*
Contact: niina.harju@uef.fi

Cigarette smoke is an environmental risk factor for age-related macular degeneration (AMD) [1]. AMD is a multifactorial disease in which, for example, retinal pigment epithelial (RPE) cells degenerate that impairing central vision [2–4]. RPE cells are essential for maintaining the functionality of photoreceptors [2,4,5]. Hydroquinone is a toxic compound in cigarettes, and it has detrimental effects on RPE cells, e.g., increasing oxidative stress, DNA damage, apoptosis, and nuclear condensation, but reduces inflammation [6,7]. These experiments aimed to study the effects of hydroquinone on mitochondria and levels of protein in ARPE-19 cells.

ARPE-19 cells (ATCC) were exposed to hydroquinone, after which total ATP and protein levels were measured. Transmission electron microscopy (TEM) was used to image mitochondria after treatments. Hydroquinone reduced total ATP and total protein levels in ARPE-19 cells. TEM images show that hydroquinone induced longer and more damaged mitochondria (Fig. 1). Hydroquinone has the properties to disrupt total cellular protein levels as well as mitochondrial function and morphology in ARPE-19 cells. More studies are needed to see the exact effects of hydroquinone on energy metabolism, such as mitochondrial function and dynamics, as well as protein synthesis.

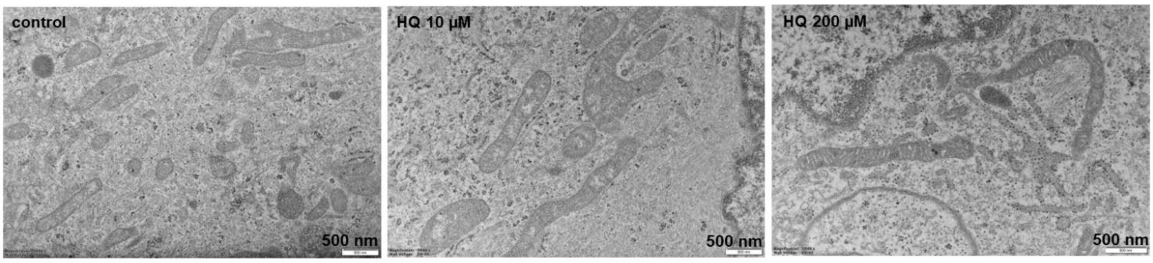


Figure 1: The effect of hydroquinone on mitochondria, illustrated by TEM.

Acknowledgment
I warmly acknowledge, especially the UEF Immuno-ophthalmology group, but also the UEF Ophthalmology group, for supporting me with reagents and cell experiments. I also acknowledge Jari Leskinen and the UEF Cell and Tissue Imaging Unit, University of Eastern Finland, Biocenter Kuopio, and EuroBioimaging Finland for assistance, guidance, and TEM imaging.

References

[1] J.C Khan, *Br J Ophthalmol.* **90**, 1, (2006).
[2] K. Kaarniranta et al. *J Alzheimers Dis.* **24**, 4, (2011).
[3] J. Blasiak et al. *Oxid Med Cell Longev.* **2017**, (2017).
[4] K. Kaarniranta et al. *Prog Retin Eye Res.* **79**, (2020).
[5] K. Kaarniranta et al. *Front Biosci (Elite Ed)*. **2**, 4, (2010).
[6] K.M. Bertram et al. *Am J Physiol Cell Physiol.* **297**, 5, (2009).
[7] N. Bhattarai et al. *Int J Mol Sci.* **21**, 2066, (2020).

Poster 10

Machine Learning-Assisted Clustering of Amino Acids: The Development of an Interaction Model of the Protein-Nanocluster Interface

Brenda Ferrari[1], Zohreh Fallah[2], Maya Khatun[2], Hannu Häkkinen[1,2]

[1]*Department of Chemistry, Nanoscience Center, University of Jyväskylä*
FI-40014 Jyväskylä, Finland
[2]*Department of Physics, Nanoscience Center, University of Jyväskylä,*
FI-40014 Jyväskylä, Finland
Contact: brenda.d.desouzaferrari@jyu.fi

The interactions that occur in the interface of proteins and ligand-stabilised metal nanoclusters (MNCs) are crucial to understanding the adsorption process of biomolecules on the surface of these nanomaterials. Despite the relevance of the adsorption phenomena for biological applications, such as bioimaging, biosensing and targeted drug delivery [1], efforts to model the interactions observed in the interface of those systems are still scarce in the literature. In this work, a model of the interactions observed in the peptide-Au$_{38}$(p-MBA)$_{24}$ interface was developed, employing clustering analysis, an unsupervised machine learning technique. The accuracy of this model was evaluated by simulating the peptide-Au$_{38}$(p-MBA)$_{24}$ interactions using Molecular Dynamics (MD) simulations and Density Functional Theory (DFT) calculations. In accordance with findings reported in the literature [2], the insights derived from this model can also be applied to the context of protein-AuNC interactions, supported by the fact that the model was developed to provide a generalisable approach. The developed model was able to predict that amino acids arginine (R), histidine (H), lysine (K), proline (P), glycine (G) and tryptophan (W) have a higher tendency of interacting with Au$_{38}$(p-MBA)$_{24}$, while aspartic acid (D) and glutamic acid (E) have a lower tendency of interacting with the same structure (Figure 1). The most prevalent interaction modes observed include the guanidine and NH_3^+ groups interacting deeper in the ligand layer and nitrogen atoms interacting in different ranges with the ligand layer and gold core atoms. Conversely, peptides with a high number of carboxylate groups interact poorly or not interact at all. The results obtained in this work can lead efforts to accelerate discoveries in the fields that rely on understanding the interactions observed at protein-AuNC interface, as it would allow the screening of a library of nanoclusters and biomolecules without depending on large batches of physical-chemical simulations.

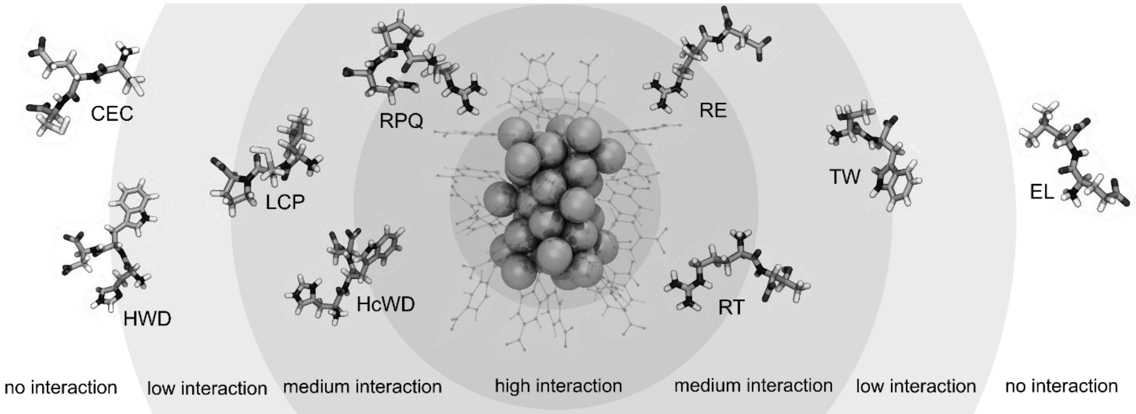


Figure 1: An illustrative representation of the order of interaction of the peptides containing two and three amino acids with Au$_{38}$(p-MBA)$_{24}$.

References:
[1] van de Looij, Sanne M., et al. Bioconjugate Chem. 33, 1, 4–23 (2022)
[2] Zhang, Bihan, et al. J. Am. Chem. Soc. 147, 8, 6404–6414 (2025)

Poster 11

Harnessing Multi-Stranded Helices for Molecular Links, Knots and Topological Hydrogels

Louise Miton[1], Dimitri Delcourt[1], Fabien B. L. Cougnon[1]
[1]*Department of Chemistry and Nanoscience Center, University of Jyväskylä, P.O. Box 35, FI-40014 JYU, Finland*
Contact: louise.l.miton@jyu.fi

Natural biomolecules such as DNA can switch between single-, double-, and triple- helical conformations to regulate their functions. Synthetic multi-stranded helices [1-2] can also exhibit dynamic features and provide a powerful platform for designing topologically complex architectures [3]. Our group has recently designed an oligo(*m*-phenylene ethynylene) strand that self-assembles into higher-order helices in aqueous environments. This amphiphilic strand, composed of hydrophobic phenylene residues and hydrophilic pyridinium groups, preferentially forms double and triple helices to minimize hydrophobic exposure and avoid electrostatic repulsion. The equilibrium between these helices is concentration-dependent, with the triple helix becoming predominant at higher concentrations. In this work, we use these helices as a scaffold towards molecular links, knots and entangled soft materials. Several new features were introduced to reach this goal. First, we introduced terminal reactive groups to either: (1) connect the upper and lower rims of the helix and form discrete molecular links or knots; or (2) cross-link multiple helices with PEG-based linkers to form 3D entangled polymer networks [4]. Then, we introduced chiral side chains to control the helicity of the structures. This work will notably help us understand how the presence of entanglements can influence hydrogel morphology and mechanical properties.

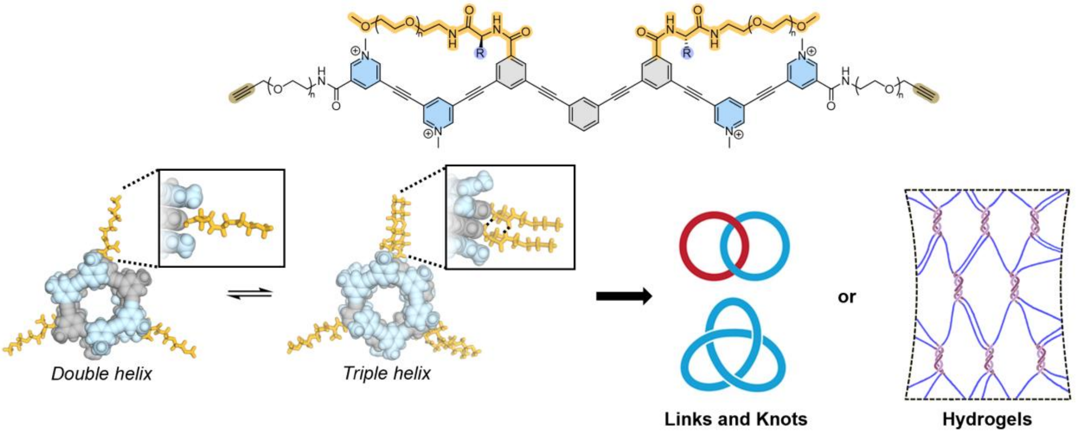


Figure 1: Schematic overview from helical self-assembly to molecular links, knots, and entangled materials.

References

[1] Hill, D. J.; Mio, M. J.; Prince, R. B.; Hughes, T. S.; Moore, J. S. *Chem. Rev.* **2001**, *101*, 3893-4012.

[2] Shang, J.; Gan, Q.; Dawson, S. J.; Rosu, F.; Jiang, H.; Ferrand, Y.; Huc, I. *Org. Lett.* **2014**, *16*, 4992-4995.

[3] (a) Ashbridge, Z.; Kreidt, E.; Pirvu, L.; Schaufelberger, F.; Stenlid, J. H.; Abild-Pedersen, F.; Leigh, D. A. *Science* **2022**, *375*, 1035-1041. (b) Carpenter, J. P.; McTernan, C. T.; Greenfield, J. L.; Lavendomme, R.; Ronson, T. K.; Nitschke, J. R. *Chem* **2021**, *7*, 1534-1543. (c) Caprice, K.; Aster, A.; Cougnon, F. B. L.; Kumpulainen, T. *Chem. Eur. J.* **2020**, *26*, 1576-1587.

[4] (a) Kim, J.; Zhang, G.; Shi, M.; Suo, Z. *Science* **2021**, *374*, 212-216. (b) Liu, C.; Morimoto, N.; Jiang, L.; Kawahara, S.; Noritomi, T.; Yokoyama, H.; Mayumi, K.; Ito, K. *Science* **2021**, *372*, 1078-1081.

Poster 12

Mammalian optogenetic tool utilizing bacteriophytochrome-based two-component signaling

Vilma Tarkiainen[1], Mervi Hyvönen[1], Kimmo Lehtinen[1], Heikki Takala[1]
[1]Department of Biological and Environmental science, University of Jyväskylä, Seminaarinkatu 15, 40014 Jyväskylän yliopisto, Finland
Contact: vilma.a.a.tarkiainen@jyu.fi

In optogenetics, complex biological processes are controlled with light, which makes this method spatiotemporally accurate and non-invasive. We have previously generated an optogenetic pREDusk tool that enables red light-induced downregulation of target gene expression in bacteria [1]. Its function stems from a bacteriophytochrome-based histidine kinase (DrF1) and an associated two-component signaling system. Here, we have transplanted this system to mammalian context, resulting in a mREDusk tool that enables over hundred-fold downregulation of target gene expression in mammalian cells with red light. By modifying its DrF1 component, we have been able to generate also red- and far-red light-activatable variants of the tool.

Breast cancer is the most common cancer worldwide in women and has still several subtypes without effective treatment. To address this, our next aim is to engineer tools to fight breast cancer with red/far-red light. To this end, we will harness the mREDusk to induce production of pro-apoptotic proteins, and hence apoptosis, in response to red/far-red light. The tools will target especially triple negative breast carcinoma cells and will be assayed in both 2D and 3D cell models. Once successful, our optogenetic apoptosis tools will pose an alternative, non-invasive option for currently used cancer therapies.

References

[1] E. Multamäki, *et al., ACS Synth Biol* **11**, 3354–3367 (2022).

Poster 13

Cloud point extraction of pyridine *N*-oxides using water-soluble calix[4]pyrroles

Julia Naulapää[1], Aliisa Kangas[1], Teppo Leino[1], Paula Perea Perez[1], Kaisa Helttunen[1]
[1]*Department of Chemistry, Nanoscience Center, University of Jyväskylä, Survonkatu 9, 40014, Finland*
Contact: jupipana@jyu.fi

Triton X-100 and Tergitol 15-S-7 are non-ionic surfactants, which form micelles in the aqueous phase. At the cloud point temperature, the micelles aggregate due to decreased hydration, causing the solution to become turbid as a result of phase separation. The separation of the micelle-rich coacervate phase from the supernatant has been utilized to extract analytes from the bulk solution. For example, cloud point extraction (CPE) has been applied in the analysis[1,2] and removal[3] of various organic and inorganic analytes. Supramolecular hosts, such as calix[n]arenes have been used to enhance the CPE of inorganic cations from solution.[4]

Calix[4]pyrroles are supramolecular hosts that belong to a class of macrocyclic porphyrinogens and bind hydrogen bond accepting guests in their cavity (Fig 1a).[5] Lately, great strides have been taken to solubilize calix[4]pyrroles in aqueous solutions to better align with the principles of green chemistry. The water-solubility has been mainly achieved by attaching ionic groups as substituents in the calix[4]pyrrole framework. Calix[4]pyrroles have been shown to bind strongly with pyridine *N*-oxides in organic solvents and water. Pyridine *N*-oxides are formed by oxidation of pyridine, and they are used as reactive intermediates in the synthesis of pharmaceuticals.[6]

We present the synthesis of novel PEGylated water-soluble calix[4]pyrroles, their host-guest properties with selected pyridine *N*-oxides and the subsequent cloud point extraction of pyridine *N*-oxide from aqueous solution with surfactant/calix[4]pyrrole mixed micelles (Fig. 1b). In the absence of a supramolecular host the surfactants Triton X-100 and Tergitol 15-S-7 are not capable of extracting pyridine *N*-oxide from the aqueous solution. With the addition of PEGylated calix[4]pyrrole into the solution, the extraction efficiency of the system can be brought up to 87 %. To the best of our knowledge, this is the first example of a host-guest chemistry aided CPE of an organic analyte.

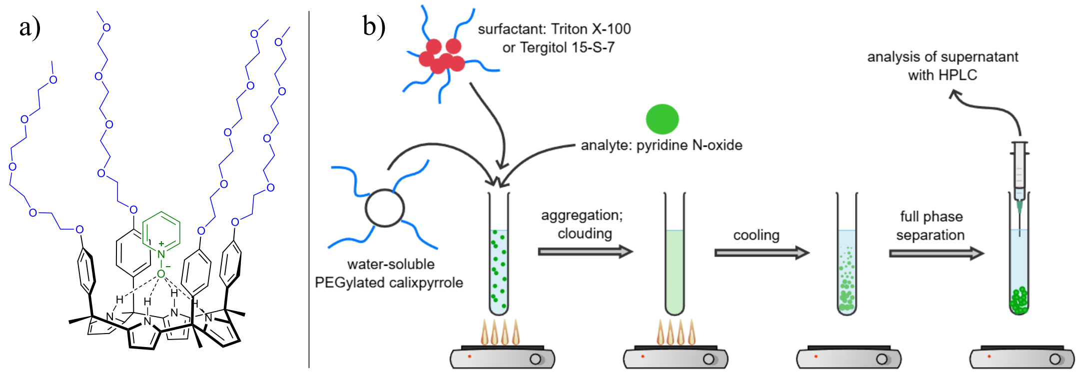


Fig 1a) Binding of pyridine *N*-oxide into the cavity of a PEGylated calix[4]pyrrole, and b) the cloud point extraction of pyridine *N*-oxide with calix[4]pyrrole and surfactant. CPE diagram was created with Chemix.

References

[1] R. Carabias-Martinez, *et al.*, *J. Chromatogr.*, **902** (2000)
[2] H. Ma, *et al., J. Sep. Sci.,* **35** (2012)
[3] M. K. Purkait, *et al., Water Res.*, **39** (2005)
[4] A. Mustafina, *et al., Talanta*, **68** (2006)
[5] P. A. Gale and J. L. Sessler, *Coord. Chem. Rev.*, **222** (2001)
[6] I. Habib, K. Singha and M. Hossain, *ChemistrySelect*, **8** (2023)

Poster 14

Electronic and Optical Properties of Metal-Ion-Mediated Au_{25} Nanocluster-Based Assemblies

Hanna Jääskö[1], Sami Malola[1], Hannu Häkkinen[1,2]
[1]*Department of Physics, Nanoscience Center, University of Jyväskylä, Jyväskylä 40014, Finland*
[2]*Department of Chemistry, Nanoscience Center, University of Jyväskylä, Jyväskylä 40014, Finland*
Contact: hanna.e.jaasko@jyu.fi

Cluster-assembled materials constructed from atomically precise noble metal nanoclusters are emerging as promising platforms for applications in nanoelectronics, sensing and bio imaging. Their electronic and optical properties can be finely tuned by changing the protecting ligands or the metal core. Linking the nanoclusters through metal ions provides an additional way to control intercluster interactions, as the choice of the metal ion determines the intercluster distances [1].

Recently, we investigated the electronic properties of two such assemblies, Au_{25}–Mg and Au_{25}–Cu, using density functional theory (DFT) [2]. These systems were found to have semiconductor-like electronic band structures, in good agreement with experimental observations. In the present work, we extend this study to the optical properties of the same materials using linear-response time-dependent DFT (LR-TDDFT). Our results show that variations in intercluster distances significantly affect both the absorption and circular dichroism (CD) spectra.

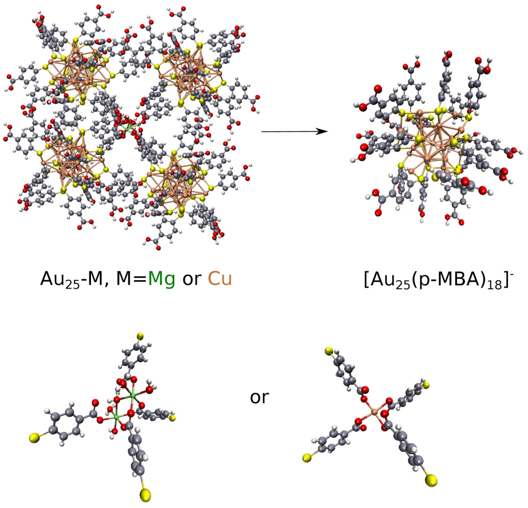


Figure 1: $[Au_{25}(p\text{-}MBA)_{18}]^-$ clusters connected via Mg or Cu atoms, leading to different types of cluster assemblies.

References

[1] Kim, Sinhyeop et al., Au25 Cluster-Based Atomically Precise Coordination Frameworks and Emission Engineering through Lattice Symmetry, ACS Nano, 18, 29036-29044 (2024)

[2] Kim, Sinhyeop et al. Tuning the Electrical Properties through Metal-Ion-Mediated Assembly in Au25 Nanocluster-Based Frameworks , *J. Am. Chem. Soc.*, 147, 34, 30803–30808 (2025)

Poster 15

Solvent-induced gelation: Effect of terminal functionality

Henna Rahkola[1], Efstratios D. Sitsanidis [1] and Maija Nissinen[1]
[1]Department of Chemistry, Nanoscience Center, University of Jyväskylä, PO Box 35, FI-40014, Finland
Contact: henna.t.k.rahkola@jyu.fi

In general, solvents do not participate actively in self-assembly processes of gelators. Instead, they are passively encapsulated within the gel network formed by the gelators. We have introduced a solvent-induced gelation (SIG) mechanism, where the solvent is chemically active and participates in the formation of organogels.[1-3] For example (Figure 1a), the precursor gelator (BocFFO*t*Bu) is selectively deprotected under acidic conditions in the presence of *tert*-butyl acetate solvent (*t*BuOAc). The Boc group of the dipeptide is irreversibly deprotected, followed by the reversible deprotection of the *tert*-butyl (*t*Bu) ester. The reaction pathway forms two gelators, which interconvert through a hydrolysis-esterification reaction cycle due to the alcohol (*tert*-butanol) formed during the hydrolysis of the solvent.[1-2]

The efficacy of SIG is assessed on several di- and tripeptide precursor gelators using different solvents.[2-3] The research has been extended to dipeptides with different terminal esters, methyl and isopropyl. Their gel-forming ability and the functionality of the SIG mechanism are investigated in solvents containing the corresponding group with ester (methyl acetate and isopropyl acetate). In addition, tests on how different solvent-donating groups affect the systems are planned. (Figure 1b).

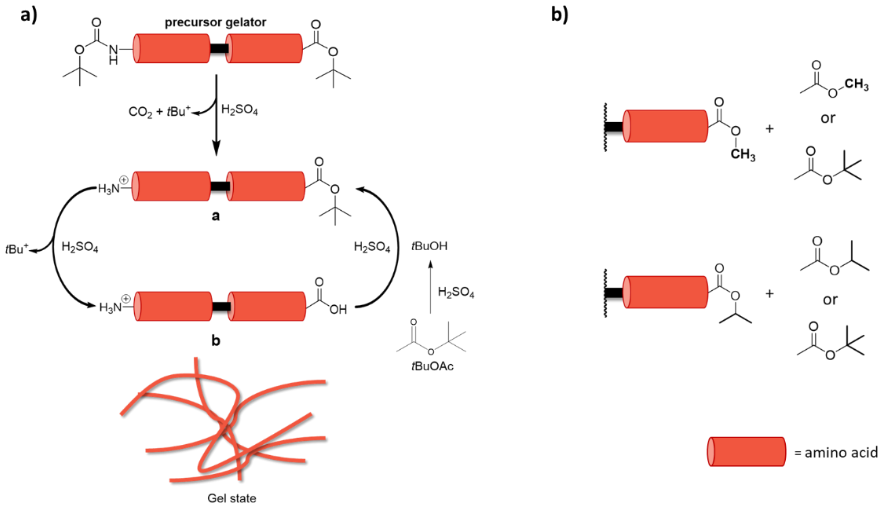


Figure 1: a) General schematic presentation of solvent-induced gelation mechanism and b) dipeptide and solvent combinations used in terminal functionality studies.

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, and M. Nissinen, *manuscript*.

Organic excitonic nanostructures for weak and strong coupling

Arpan Dutta[1], J. Jussi Toppari[1]
[1]*Nanoscience Center and Department of Physics, University of Jyväskylä, P.O. Box 35, FI-40014, Finland*
Contact: arpan.a.dutta@jyu.fi

Organic excitonic nanostructures exhibit Frenkel excitons at room temperature with high absorption and are a promising alternative for plasmonic systems. These excitonic materials are derived from organic dye-doped polymer films by increasing the doping concentration so much that the real part of the permittivity goes negative, i.e., $\mathrm{Re}\{\epsilon(\omega)\} < 0$, within an energy range just above their material absorption. Within this narrow band of negative-real-permittivity, the organic film supports surface exciton (SE) modes analogous to the surface plasmon (SP) modes in metals [1,2]. Like SP modes, SE modes can be exploited in refractive index sensing and near-field enhanced spectroscopy in the weak coupling regime [3] and as an optical cavity in the strong coupling regime [4]. In this work, we report how to enhance the optical performance of the SE modes by optimizing the choice of excitonic dyes as well as their doping concentration and how they can be utilized as the resonator mode for the strong coupling applications. We study the effect of molecular concentration in terms of oscillator strength (f) and Lorentzian broadening (γ) on various SE modes when employed in sensing and spectroscopy and whether SE modes can strongly couple to the photoactive molecules and SP modes or not. Our simulations reveal that, in the weak coupling regime, the optical performance of an excitonic system is tunable via molecular concentration, while, in the strong coupling regime, SE modes can facilitate strong coupling by sustaining energy-splitting-induced transparency. However, polaritons may not be visible in absorption since they can easily be located outside of the narrow energy range of negative real permittivity. Our findings shed light on the weak and strong coupling properties of SE modes for contemporary organic nanophotonics.

References

[1] L. Gu, *et al.*, *Appl. Phys. Lett.* **103**, 021104 (2013).
[2] M. J. Gentile, *et al.*, *Nano Lett.* **14**, 2339 (2014).
[3] A. Dutta and J. J. Toppari, *Opt. Mater. Express* **13**, 2426 (2023).
[4] A. Dutta and J. J. Toppari, *Phys. Rev. B* **109**, 165117 (2024).

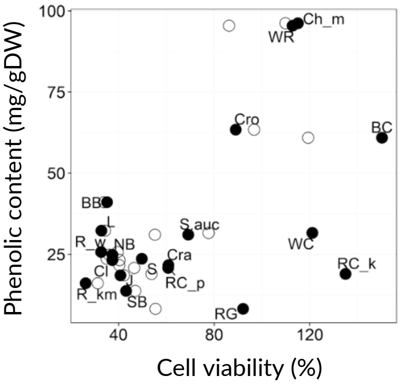
Poster 17

Antibacterial and antiviral properties of Finnish berries

Yomi Matsumoto-Viljanen[1], Anniina Runtuvuori-Salmela[2], Daniel de Oliveira[2], Miika Karjalainen[2], Laura Myllymäki[2], Lotta-Riina Sundberg [2], Varpu Marjomäki[2], and Kaisa Helttunen[1]
[1]*Department of Chemistry, Nanoscience Center, University of Jyväskylä, Finland*
[2]*Department of Biological and Environmental Science, Nanoscience Center, University of Jyväskylä, Finland*
Contact: yomi.j.matsumoto-viljanen@jyu.fi

Natural biomaterials are important in Finland's bioeconomy and Finland has a particularly abundant supply of berry resources. Many berries are used in foods, cosmetics, and the pharmaceutical industry. Berries' functional properties such as antioxidant, anti-inflammatory, anticancer, and other bioactive properties have been studied over the years [1,2]. However, there is still much room for research on antibacterial and antiviral properties, especially against enteroviruses and human coronaviruses that cause hand, foot, and mouth disease, and respiratory tract infections. In this study, we conduct comprehensive antiviral and antibacterial screening on approximately 20 different wild and cultivated berries. We aim to discover new values of berries, specifically their antibacterial and antiviral effects, and to elucidate the compounds responsible for these activities.

A general profiling of compounds in the berry extracts was performed using HPLC-DAD, which revealed flavonols and anthocyanins in many berry extracts. Total phenolic content of the extracts was determined as gallic acid equivalents (GAE) using Folin-Ciocalteu method,[3] and anthocyanin content was determined with pH differential method.[4] Correlation between these contents and the antiviral activities against human coronaviruses were evaluated (Figure 1). The correlation analysis revealed a statistically significant relationship between both phenolic content and anthocyanin content with antiviral activities, where the variance in the antiviral activity explained by the phenolic content was stronger with lower extract concentrations.



Concentration of berry extracts	R^2	p_value
● = 10 mg/mL	0.52	0.02
○ = 5 mg/mL	0.78	9.0×10^{-5}

Figure 1: The correlation between phenolic content (GAE) and antiviral efficacy of the berry extracts against human coronaviruses.

References

(1) Baby, B.; Antony, P.; Vijayan, R. Antioxidant and Anticancer Properties of Berries. *Crit. Rev. Food Sci. Nutr.* **2018**, *58* (15), 2491–2507. https://doi.org/10.1080/10408398.2017.1329198.

(2) Pap, N.; Fidelis, M.; Azevedo, L.; do Carmo, M. A. V.; Wang, D.; Mocan, A.; Pereira, E. P. R.; Xavier-Santos, D.; Sant'Ana, A. S.; Yang, B.; Granato, D. Berry Polyphenols and Human Health: Evidence of Antioxidant, Anti-Inflammatory, Microbiota Modulation, and Cell-Protecting Effects. *Curr. Opin. Food Sci.* **2021**, *42*, 167–186. https://doi.org/10.1016/j.cofs.2021.06.003.

(3) Singleton, V. L.; Orthofer, R.; Lamuela-Raventós, R. M. [14] Analysis of Total Phenols and Other Oxidation Substrates and Antioxidants by Means of Folin-Ciocalteu Reagent. In *Methods in Enzymology*; Oxidants and Antioxidants Part A; Academic Press, 1999; Vol. 299, pp 152–178. https://doi.org/10.1016/S0076-6879(99)99017-1.

(4) Lee, J.; Durst, R. W.; Wrolstad, R. E.; Collaborators: Determination of Total Monomeric Anthocyanin Pigment Content of Fruit Juices, Beverages, Natural Colorants, and Wines by the pH Differential Method: Collaborative Study. *J. AOAC Int.* **2005**, *88* (5), 1269–1278. https://doi.org/10.1093/jaoac/88.5.1269.

Poster 18

Increasing the domain size of DNA origami lattices on silicon

H. Järvinen[1], J. M. Parikka[1], R.P.T.N. Rajapaksha[1], A. Keller[2] and J. J. Toppari[1]
[1]*Department of Physics and Nanoscience Center, 40014 University of Jyväskylä, Finland*
[2]*Technical and Macromolecular Chemistry, Paderborn University, 33098 Paderborn, Germany*
Contact: rptnraja@jyu.fi

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].

Cross-shaped DNA origami can be used as building blocks, *i.e.*, tiles to form fishnet-type lattices on a substrate. When combined with methods such as DNA assisted lithography (DALI) [5] one can obtain metasurfaces. Earlier, we have developed a large-scale fabrication methodology to produce a closely spaced two-dimensional fishnet-type lattices on a silicon substrate [3]. Similar lattices have been formed on the common mica substrate [4], but the importance of silicon is that it allows further nanofabrication processes, such as metallization or lithography [5]. This formed polycrystalline lattice on silicon has high surface coverage and is extendable to the wafer scale with an average domain size of about a micrometer as shown in the AFM image of Figure 1a [3].

Here, the assembly of the polycrystalline lattice on silicon has been further optimized to double the average domain size [6]. It is essential to grow the domain size toward a fully single-crystalline large lattice to further advance the optical response obtained from the corresponding metallized metasurface. Wider testing of different ionic environments and concentrations were conducted as well as tuning of the tile-tile bonding strength via the number of blunt end interactions. So far, we have succeeded in enhancing lattice formation by doubling the domain size to ~2 μm as shown in the AFM image of Figure 1b.

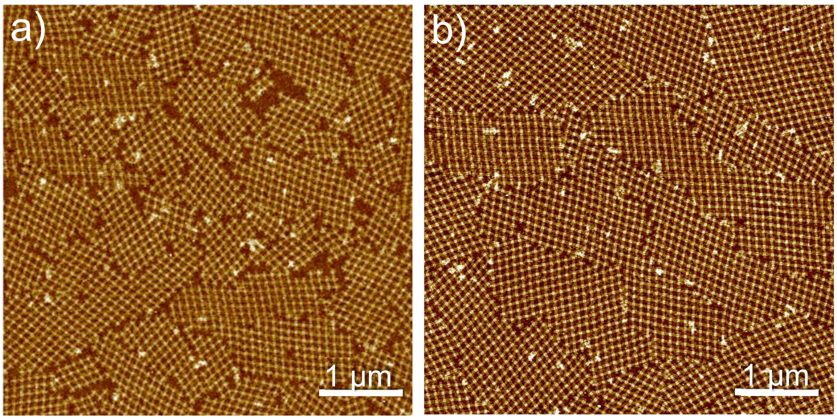


Figure 1: Atomic force microscope (AFM) images of DNA origami fishnet-type lattice on silicon with the average domain size of a) 1 μm [3] and b) ~2 μm [6].

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, et al., *Chem. Mater.* **35**, 1961-1971 (2023).
[4] J.M. Parikka, K. Sokołowska, N. Markešević, and J.J. Toppari, *Molecules* **26**, 1502 (2021).
[5] B. Shen, V. Linko, K. Tapio, *et al. Sci. Adv.* **4**, eaap8978 (2018).
[6] H. Järvinen, J.M. Parikka, R.P.T.N. Rajapaksha, A. Keller, and J.J. Toppari, *"Increasing the domain size of DNA origami lattices on silicon" In preparation, to be submitted to Small Structures*

Poster 19

Floquet-engineering heat pulses in one-dimensional wires

Pedro Portugal[1], Riku Tuovinen[2], Christian Flindt[1]
[1]*Department of Applied Physics, Aalto University, Finland*
[2]*Department of Physics, Nanoscience Center, University of Jyväskylä, Finland*
Contact: pedro.decastroportugal@aalto.fi

A Floquet scattering theory of heat pulses in ballistic conductors was recently developed [1], enabling the modeling of time-dependent temperature gradients in ultrafast and ballistic electronics using Luttinger fields [2]. In that framework, heat pulses were simulated in electron quantum optics setups such as the Hong–Ou–Mandel experiment, where both bunching and antibunching of the generated excitations were observed.

Direct implementation of these fields, however, is challenging, as it would require dynamically tuning the Fermi velocity. In forthcoming work [3], we address this difficulty by proposing a Floquet engineering scheme within a tight-binding model of electronic transport in one-dimensional wires. Floquet engineering employs fast and periodic external drives to manipulate system properties, including the Fermi velocity, a technique that has already been demonstrated experimentally in quantum systems such as graphene [4]. Within this setting, we analyze the heat and electric current and their fluctuations across a quantum point contact.

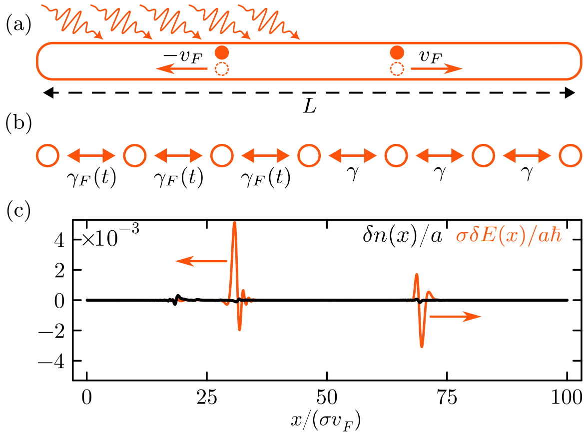


Figure 1: (a) A fast external drive generates a heat pulse, which travels along a one dimensional wire of length L with fermi velocity v_F. The excitation carries equal number of electrons and holes. (b) The wire can be modeled by a tight-binding chain with a tunneling rate $\gamma = v_F/2a$, where $a = L/N$ is the distance between each site for a chain with N sites. The drive effectively changes the tunneling rate in part of the chain to $\gamma_F(t)$. (c) Excess charge (black) and energy (orange) per site (compared to equilibrium) generated by the effective time-dependent Luttinger field.

References

[1] P. Portugal, F. Brange, and C. Flindt, Phys. Rev. Lett. **132**, 256301 (2024).

[2] J. M. Luttinger, Phys. Rev. **135**, A1505 (1964).

[3] P. Portugal, R. Tuovinen, and C. Flindt, (to be announced, 2025-6).

[4] M. Merboldt et al., Nat. Phys. **21**, 1093 (2025)

Poster 20

Josephson effect at arbitrary disorder strength in systems with generic spin-dependent fields

Maryam Darvishi[1], F. Sebastián Bergeret[2,3], and Stefan Ilić[1]

[1]Department of Physics and Nanoscience Center, University of Jyväskylä,
[2]Centro de Física de Materiales (CFM-MPC) Centro Mixto
CSIC-UPV/EHU, E-20018 Donostia-San Sebastián, Spain
[3]Donostia International Physics Center (DIPC), 20018 Donostia–San Sebastián, Spain

September 8, 2025

Abstract

We present a theory of the Josephson current in superconductor-normal metal-superconductor (SNS) junctions in the presence of generic spin-dependent fields, such as spin-orbit coupling (SOC), Zeeman fields, and altermagnetism. We consider systems with arbitrary disorder strength, going beyond the usual diffusive and ballistic approximations. Using the linearized quasiclassical Eilenberger equation, we derive a compact expression for the Josephson current, which is then applied to various situations of experimental interest. First, we investigate the evolution of the Josephson current in the presence of several types of SOC and an applied Zeeman field. In particular, we discuss the anomalous Josephson effect (φ_0) in systems linear-in-momentum SOC, and demonstrate that the effect is present in a wide window of disorder strength. Second, we investigate the Josephson current in disordered junctions with altermagnets, and show how the $0-\pi$ transition in such systems is rapidly suppressed by disorder. Our results may be useful for describing experimental setups with high-mobility samples, which nevertheless always contain some amount of disorder. For such systems, neither ballistic nor diffusive approximations are appropriate, and one needs to use a more general theory provided by our work.

Contact: maryam.m.darvishi@jyu.fi

Poster 20

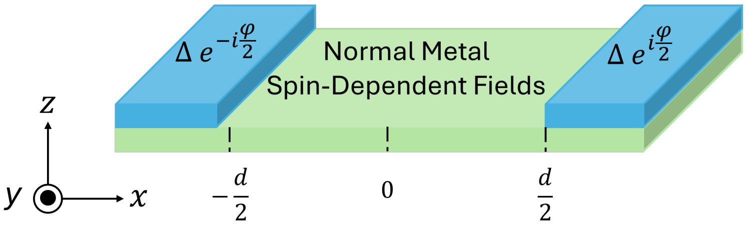


Figure 1: Schematic illustration of the SNS junction with spin-dependent fields and disorder.

Poster 21

PDMS as a flexible substrate for graphene biosensors

Virginia Ranaweera[1], Mika Pettersson[1], Andreas Johansson[1,2]
[1]Department of Chemistry, [2]Department of Physics, Nanoscience Center, University of Jyväskylä,
Survontie 9C, 40500 Jyväskylä, Finland
Contact: virginia.m.ranaweera@jyu.fi

PDMS was assessed for its suitability as a flexible substrate for graphene devices, along with a novel fabrication method that supports the transfer of CVD graphene directly, without the need for a support film such as PMMA. This approach enables the utilization of PDMS as a functional substrate [1].

Experimental work included spin-coating of PDMS [2] on CVD graphene, followed by etching of the metal catalyst to obtain a graphene /PDMS stack. The success of the process and the quality of the graphene were affirmed by AFM and Raman spectroscopy, which indicated the presence of high-quality single-layer graphene on PDMS by the high I_{2D}/ I_G ratio.

The graphene on PDMS was functionalised by two-photon oxidation [3] to enhance the compatibility in mimicking biological environments. AFM data indicated minimal height modifications. However, the influence of high doses on mechanical properties was evident. Raman mapping confirmed defect induction correlated with pulse energy and exposure time.

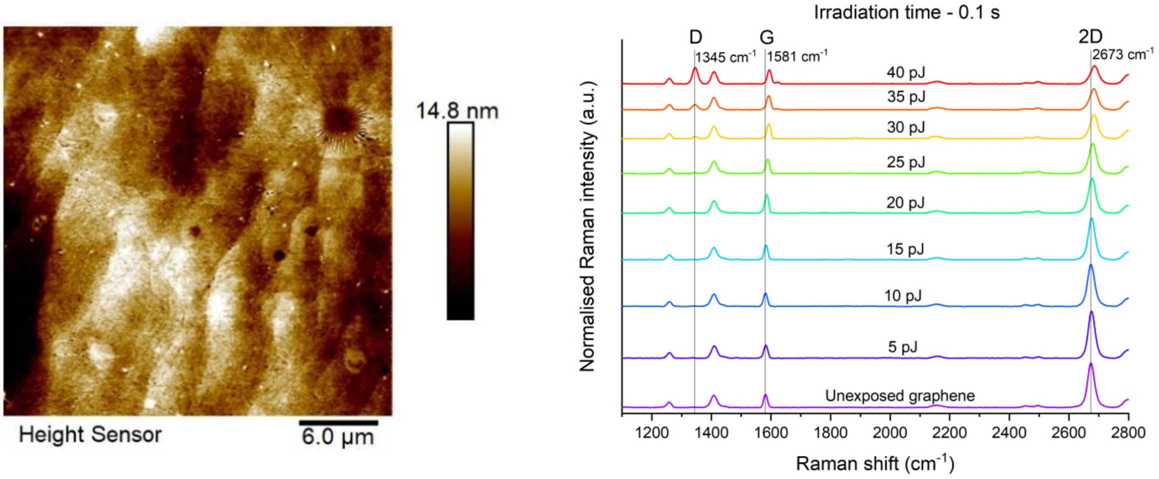


Figure 1: AFM and Raman data after 2PO of graphene on PDMS.

Graphene remained largely intact with modest defects, likely within the point defect regime. The 2D band response suggested a resonance shift due to altered interactions between graphene and PDMS. Lower pulse energy doses appeared to clean the graphene surface, whereas, beyond a threshold, the two-photon oxidation (2PO) process dominated.

The preservation of graphene on PDMS during laser exposure demonstrated its stability and behaviour comparable to graphene on SiO_2. These findings underscore the viability of PDMS as a functional flexible substrate for graphene and reinforce its potential for flexible graphene electronics.

The authors would like to acknowledge support from Jane and Aatos Erkko Foundation.

References

[1] Ullah et al., *Nano Research*, ***14***, 3756-3772, (2021).
[2] El-Molla et al., *Journal of Sensors*, *2016(1)*, 1736169, (2016).
[3] Aumanen et al., *Nanoscale*, *7*, 2851-2855, (2015).

Poster 22

Bias-Driven Electroluminescence in Molecular Junctions

Oscar A. Moreno Segura[1], and Riku Tuovinen[1]
[1]Department of Physics, Nanoscience Center, University of Jyväskylä, Jyväskylä 40014, Finland
Contact: oscar.a.morenosegura@jyu.fi

We investigate the electroluminescence effect in a molecular junction driven by a tunneling current as in a scanning tunneling microscope setup. Here, we use a time-linear nonequilibrium Green's function (NEGF) formalism [1] to study the electroluminescence of a molecule connected to two electrodes and coupled to a cavity. Our current approach treats electron–electron interactions within the molecule at the Hartree–Fock level, while electron–photon coupling is explored via the Ehrenfest approximation. We focus on the photonic and electronic responses in order to describe the electroluminescence in the system under weak and intermediate effective couplings. Our calculations are performed with the CHEERS code [2], which implements quantum transport simulations based on NEGF.

To illustrate our framework, we apply it to the Holstein dimer model and the benzenedithiol molecule, characterizing emission mechanisms and operating regimes. Finally, we present density functional theory (DFT) results for tin phthalocyanine (SnPc), which has two geometric configurations, only one of which exhibits light emission under bias. These DFT results are the starting point for applying our Green's function framework to SnPc.

References

[1] Tuovinen, R., Pavlyukh, Y., Perfetto, E., & Stefanucci, G. (2023). Time-linear quantum transport simulations with correlated nonequilibrium green's functions. Physical Review Letters, 130(24), 246301.

[2] Pavlyukh, Y., Tuovinen, R., Perfetto, E., & Stefanucci, G. (2024). Cheers: A Linear-Scaling KBE+ GKBA Code. physica status solidi (b), 261(9), 2300504.

Poster 23

Nonequilibrium dynamics in the spin-boson model

Joona Marjamäki[1], Robert van Leeuwen[1], Riku Tuovinen[1]
[1]*Department of Physics, Nanoscience Center, P.O. Box 35, 40014 University of Jyväskylä, Finland*
Contact: joona.a.marjamaki@jyu.fi

The usual approach to studying the dynamics of an open quantum system is to use a quantum master equation (QME) with Markovian evolution and weak coupling, leading to the Redfield or Lindblad equations [1]. However, in the presence of strong coupling or a strong driving field, the Markovian time evolution may no longer be valid.

We model a qubit coupled to an environment using the spin-boson model and examine the effects of strong coupling and driving pulses on the system's dynamics. The pulses represent laser pulses used in the implementation of gate operations between qubits in quantum computers [2]. We investigate how strong coupling influences the adiabatic interaction between the system and its environment, as well as the system's behavior after being driven into a nonequilibrium state.

References

[1] H.-P. Breuer, and F. Petruccione, The Theory of Open Quantum Systems (Oxford University Press on Demand, New York, 2002).
[2] E. Pelucchi, G. Fagas, I. Aharonovich, D. Englund, E. Figueroa, Q. Gong, H. Hübel, J. Liu, C.-Y. Lu, N. Matsuda, J.-W. Pan, F. Schreck, F. Sciarrino, C. Silberhorn, J. Wang, and K. D. Jöns, Nat. Rev. Phys. 4, 194 (2022).

Poster 24

A computational exploration of photocatalytic hydrogen and oxygen evolution reaction pathways in low-dimensional Ni/MoS$_2$ systems

Aku Lempelto[1], Veera Juntunen[1], Shubo Wang[1], Takashi Yamamoto[2], Viktorija Pankratova[1], Samuli Urpelainen[1], Marko Huttula[1], Wei Cao[1]
[1]*Nano and Molecular Systems Research Unit, University of Oulu, Pentti Kaiteran katu 1, P.O.Box 8000 FI-90014, Oulu, Finland*
[2]*Department of Science and Technology, Tokushima University, Tokushima 770 8506, Japan*
Contact: aku.lempelto@oulu.fi

Photocatalytic water splitting is a promising alternative to electrolysis, as it enables the sustainable production hydrogen using nothing but sunlight and water. To this end, we may build a photocatalytic system from carefully chosen semiconductor materials and form a low-dimensional heterojunction that promotes charge separation after photon adsorption. This slows down charge recombination and thus allow hydrogen and oxygen evolution reactions to take part on the surface of the components [1,2]. Our work uses density functional theory as a computationally efficient way to explore HER/OER elementary reactions on the surface of a Ni/MoS$_2$ catalyst under photocatalytic operation.

We present a thermodynamic examination of water splitting using neutral and charged nickel oxide/hydroxide slab models. The calculations were carried out using the GPAW package. Solvation at the water-solid interface is addressed with a combination of implicit and explicit solvent models. The computational results demonstratate how the main intermediates of the HER/OER process are stabilized by photo-generated charges localized on the surfaces of nickel phases [NiO, NiO$_2$, Ni(OH)$_2$]. The results help quantify the thermodynamics of water adsorption and subsequent photocatalytic dissociation. Finally, the computational findings are combined with an extensive experimental ambient *operando* characterization, bringing a new closer look at the the evolution and interconversion of the phases in Ni/MoS$_2$ systems under light irradiation and the presence of water. Together, the results provide an improved understanding of the photocatalytic mechanisms of nickel-based photocatalysts and the chemical changes they undergo under reaction conditions.

References

[1] K. Mishra, N. Devi, S. S. Siwal, V. K. Gupta, V. K. Thakur *Adv. Sustain. Syst.* **7**, 2300095 (2023).

[2] J. Low, J. Yu, M. Jaroniec, S. Wageh, A. A. Al-Ghamdi *Adv. Mater.* **29**, 1601694 (2017).

Poster 25

Area-selective ALD as dielectric for top-gated GFET

Maryam Naderpour [1], Mika Pettersson[1], Andreas Johansson[1,2]
Nanoscience Center, [1]Department of Chemistry, [2]Department of Physics, University of Jyväskylä, P.O. Box 35, FI-40014, Finland
Contact: maryam.m.naderpour@jyu.fi

Creating a highly conformal and atomic-scale insulating layer in graphene field-effect transistors (GFETs) is crucial for achieving high sensitivity, low leakage currents, and reliable performance in sensing applications. However, the chemical inertness of two-dimensional materials like graphene significantly limits conventional deposition methods, particularly for dielectric layers. To overcome this challenge, we utilize direct femtosecond two-photon oxidation, a non-invasive and precisely controlled technique that modifies the graphene surface by introducing oxygen-containing functional groups [1]. These functionalized regions act as nucleation sites for area-selective atomic layer deposition (ALD), allowing for the growth of uniform, ultrathin insulating layers. The resulting gate dielectric is thin, conformal, and chemically stable under physiological conditions, making it highly suitable for biosensing applications. Our research shows that oxidized graphene with a dielectric ZnO layer can be reduced through subsequent annealing processes, restoring it to its pristine state [2]. We will present our findings on how to utilize this technique to fabricate graphene FET sensors.

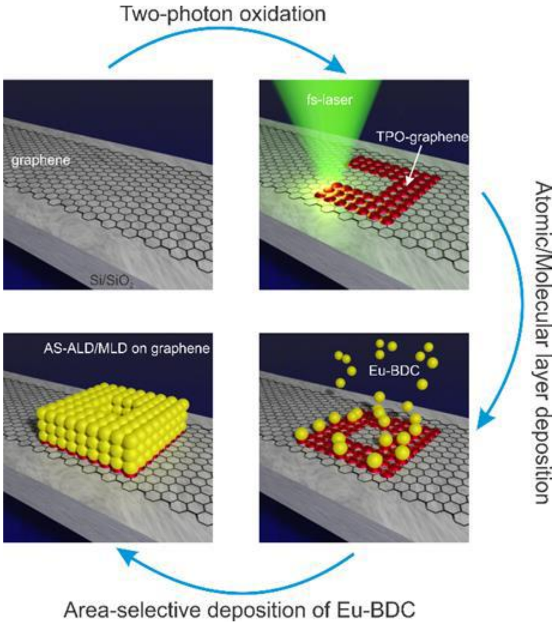


Fig. 1. Experimental scheme illustrating the femtosecond two-photon oxidation (TPO) of graphene followed by area-selective ALD/MLD of Eu-BDC thin films on predefined regions [3].

References

[1] J. Aumanen, A. Johansson, J. Koivistoinen, P. Myllyperkiö, M. Pettersson, Nanoscale, 7, 2851–2855 (2015).

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

[3] A. V. Emelianov, K. K. Mentel, A. Ghazy, Y.-H. Wang, A. Johansson, M. Karppinen, M. Pettersson, ChemRxiv, preprint, https://doi.org/10.26434/chemrxiv-2024-81qv0 (2024).

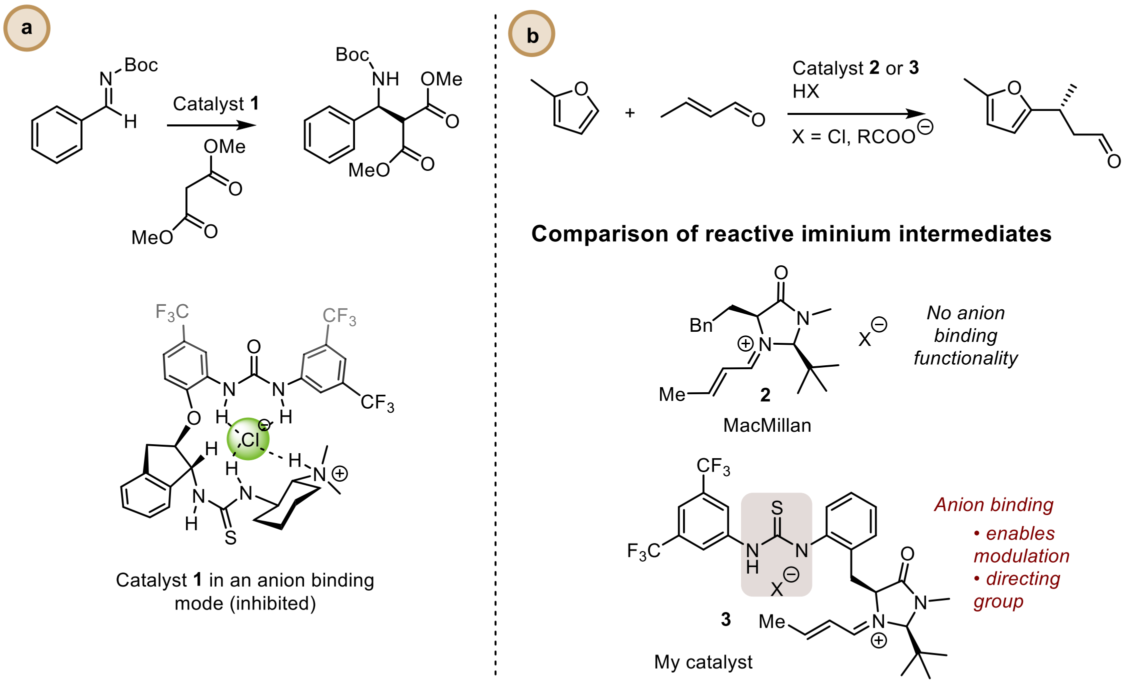
Poster 26

Anion-modulated iminium catalysts

M.Sc. Eeki Tarkkonen, Prof. Petri Pihko
[1]*Department of Chemistry, University of Jyväskylä, Survontie 9B 40500 Jyväskylä, Finland*
Contact: eejotark@jyu.fi

In our previous publication,[1] we discovered that reaction **A** with urea-thiourea catalyst **1** is efficiently inhibited by chloride ions. Furthermore, we showed that the reaction proceeds with 2nd order dependency with respect to the catalyst. These results beg the question: is it possible to develop catalysts which can be modulated or even activated by addition of an ion, instead of mere inhibition? To achieve this, new catalysts designs that incorporate both anion-binding moieties such as (thio)ureas as well as additional activating groups, such as secondary amines, are necessary.

Here we show that by modifying MacMillan's catalyst **2** with thiourea functionality, a stable iminium catalyst (**3**) is obtained which possesses both a secondary amine for iminium activation as well as a suitable anion-binding pocket (thiourea functionality). In the literature, previous attempts at combining these functionalities in the same catalyst scaffold have not been successful[2]. Experiments with the new catalyst **3** with different nucleophiles and anions will be described.



Catalyst **1** in an anion binding mode (inhibited)

Comparison of reactive iminium intermediates

No anion binding functionality

MacMillan

Anion binding
- *enables modulation*
- *directing group*

My catalyst

Scheme 1. Our previous publication showed a decrease in rate of reaction A, which cannot be explained using 1st order dependency with respect to catalyst **1**. Friedel-Crafts-reaction B with MacMillan iminiumcatalyst **2** is known. I have developed a catalyst that extends MacMillan catalyst with an anion binding moiety **3** (thiourea).

References

[1] Leino, T. O., Noutsias, D., Helttunen, K., Moilanen, J. O., Tarkkonen, E., Kalenius, E., ... & Pihko, P. M. Hypersensitive Inhibition of Organocatalysts by Halide Salts: Are Two Catalysts Involved in the Mannich Reaction?. European Journal of Organic Chemistry, **2024** 27(26), e202400321.

[2] Reyes-Rangel, G., Vargas-Caporali, J., & Juaristi, E. In search of diamine analogs of the α, α-diphenyl prolinol privileged chiral organocatalyst. Synthesis of diamine derivatives of α, α-diphenyl-(S)-prolinol and their application as organocatalysts in the asymmetric Michael and Mannich reactions. *Tetrahedron*, **2016** *72*(3), 379-391.

Poster 27

Phonon-Blocked Junction Calorimeter

Zhuoran Geng[1], Joel Hätinen[2], Emma Mykkänen[2], Renan Loreto[2], Mika Prunnila[2], Ilari Maasilta[1]
[1]Nanoscience Center, Departments of Physics, University of Jyväskylä, Finland
[2]VTT Technical Research Center of Finland Ltd., VTT Espoo, Finland
Contact: *zhgeng@jyu.fi*

Current microcalorimetry schemes face an inherent trade-off between sensitivity, needing to hold heat for a clear signal, and speed, which requires rapid heat removal to reset. We propose a phonon-blocked semiconductor–superconductor tunnel junction [1] that overcomes this limitation. By suppressing the phonon heat-flow channel [2] and using the tunneling current both as the sensing signal and as the heat-relaxation pathway, our design promises microcalorimeters performance with sensitivity and response times beyond the current state of the art [3].

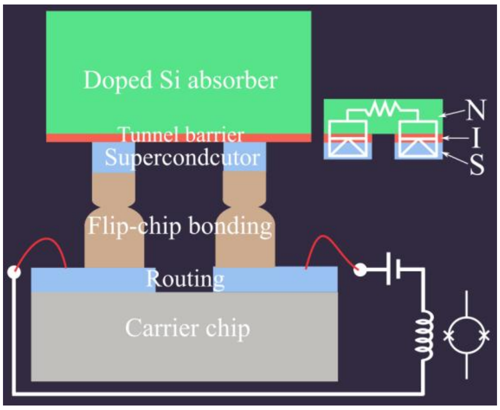


Figure 1: Schematic of a flip-chip-bonded, phonon-blocked junction microcalorimeter.

References

[1] E. Mykkänen, *et al., Sci. Adv*. **6**, eaax9191 (2020).

[2] J. Hätinen, *et al., Appl. Phys. Lett*. **123**, 152202 (2023).

[3] Z. Geng, *et al., arXiv:2508.05490* (2025).

Poster 28

A mechanical device engineered for coherent control of spin

Pooja Sudha[1], Menno Jansen[2], Ewold Verhagen[2], Juha Muhonen[1]

[1]*Department of Physics and Nanoscience Center, University of Jyväskylä, P.O. Box 35, FI-40014 University of Jyväskylä, Finland*
[2]*Centre for Nanophotonics, AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands*
Contact: psudha@jyu.fi

Silicon spin qubits combine long coherence times [1] with high-fidelity control [2] and readout [3], yet their scalability remains limited by lack of efficient coupling mechanisms that can support large-scale integration. Hybrid quantum platforms that harness mechanical or photonic devices offer a promising route to overcome this challenge [4,5]. Here, I will present our work on a phononic waveguide architecture designed, through COMSOL simulations, to enable coherent coupling with spin qubits in silicon. The proposed device integrates a high-strain phononic region optimized for spin-strain interaction, providing a mechanism for coupling spins to acoustic modes, with an adjacent phononic waveguide that can mediate long-range qubit-qubit coupling across remote spin sites. The waveguide is engineered to resonate with the spin-transition frequency of bismuth donors in silicon, ensuring compatibility with donor-based spin qubits. Our simulations demonstrate that such a hybrid design can provide a scalable pathway for coherent spin coupling, potentially enabling the construction of larger, interconnected silicon-based quantum architectures. Beyond computation, the framework additionally offers prospects for quantum sensing and transduction.

References

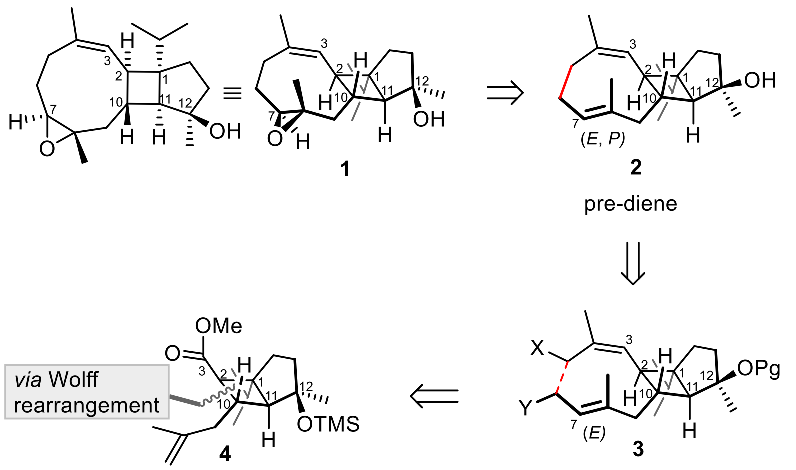
[1] J. T. Muhonen et al., *Nature Nanotech* **9**, 12 (2014).
[2] J. T. Muhonen et al., *J. Phys.: Condens. Matter* **27**, 154205 (2015).
[3] A. Morello et al., *Nature* **467**, 7316 (2010).
[4] Y. Chu et al., *Science* **358**, 199 (2017).
[5] A. Bienfait et al., *Science* **364**, 368 (2019).

Poster 29

Towards total synthesis of humilisin E: Finding strategies for construction of the 9-membered ring

M. Sc. Aino Rolig, Prof. Petri Pihko
Department of Chemistry, University of Jyväskylä, Survontie 9B, 40500 Jyväskylä, Finland
Contact:aino.m.rolig@jyu.fi

Humilisin E (**1**) is a novel diterpenoid isolated from the South China Sea, soft coral *Sinularia Humilis* [1]. It is comprised of a highly substituted cyclobutene ring fused together with a cyclopentane and cyclononene ring systems. The fused ring structure containing several stereocenters and the presence of a 9-membered ring with different functionalities make it an interesting target for total synthesis. We have previously reported the stereoselective synthesis of the bicyclic core (**4**) involving Wolff rearrangement as key step [2]. As an ongoing challenge, we are trying to explore synthetic strategies for making the 9-membered ring of humilisin E. The potential precursor for **1** could be the corresponding (3*Z*, 7*E*)-diene **2**. The (*P*)-atropisomer of **2** possesses a configuration that leads to **1** via epoxidation of the (7*E*) alkenyl group. Employing this strategy requires the construction of a fused cyclononadiene. Despite the importance of 9-membered rings in natural products and medicinally important compounds, their synthesis still often requires specific strategies to enable the cyclization step [3]. Since synthesis of such structures is known to be challenging due to the inherent strain in them, we have also approached the problem by using a model compound to explore possible synthetic strategies. Aspects of the synthetic strategies, current progress and plans towards closing of the 9-membered ring of humilisin E will be presented.



conformational freedom of the C2 and C10 side chains should be restricted by the rigid cyclobutane ring

Figure 1: Possible synthetic strategy for closing the 9-membered ring of humilisin E.

References

[1] L. L. Sun, W. S. Li, J. Li, H. Y. Zhang, L. G. Yao, H, Luo, Y. W. Guo, and X. W. Li, *J.Org. Chem.* **86**, 4, 3367-3376 (2021).

[2] P. Verma, R. R. Pallerla, A. Rolig, and P. M. Pihko, *J. Org. Chem.* **89**, 10, 6987-6990 (2024).

[3] A. K Clarke and W. P. Unsworth, *Chem. Sci.* **11**, 2876-2881 (2020).

Poster 30

Investigation of $Au_{22}KCK_{16}$ Nanocluster and Reactive Oxygen Species (ROS)

Işılay Öztürk,†[1], Lily Arrue Ayala†[1], María Matus Cortés[1], Sami Malola[1], Hannu Häkkinen[1]
Departments of Physics and Chemistry, Nanoscience Center, University ofJyväskylä, Jyväskylä FI-40014, Finland
Contact: isilay.i.ozturk@jyu.fi, lily.c.arrueayala@jyu.fi

Ligand-protected gold nanoclusters ($Au_{22}(SR)_{16}$) display unique structural and optical properties, with strong potential in catalysis, sensing, and bioimaging [1,2]. Their response, however, is highly sensitive to environmental factors such as charge, pH, and ligand chemistry [3]. In this study, we employ a multiscale approach combining long-timescale molecular dynamics (MD) simulations with Density Functional Theory (DFT) and Time-Dependent DFT (TDDFT) to investigate the interplay between conformational stability, electronic excitations, and functional group reactivity of $Au_{22}(SR)_{16}$ in aqueous environments.

MD simulations reveal distinct conformational populations and water-dependent ligand arrangements, particularly involving lysine side-chain amino groups and cysteine thiols. Analysis of these groups highlights their dual role: amino groups influence electrostatic stabilization and potential proton-transfer pathways, while cysteine thiols represent the most reactive sites for electron transfer, disulfide formation, and reactive oxygen species (ROS) generation [2,4]. TDDFT absorption spectra further demonstrate charge- and pH-dependent shifts in the UV–visible region, consistent with experimental observations [1,3].

By connecting conformational dynamics, functional group chemistry, and electronic excitations, this work provides an integrated view of how ligand environments shape the spectroscopic and reactive behavior of $Au_{22}(SR)_{16}$. The results highlight the critical role of lysine side chains in electrostatic stabilization and proton transfer, and cysteine thiols as the dominant reactive sites for electron transfer and ROS generation. These insights advance the design of ligand-engineered gold nanoclusters as tunable platforms for bioimaging, ROS-mediated therapy, and nanoscale sensing [1–5].

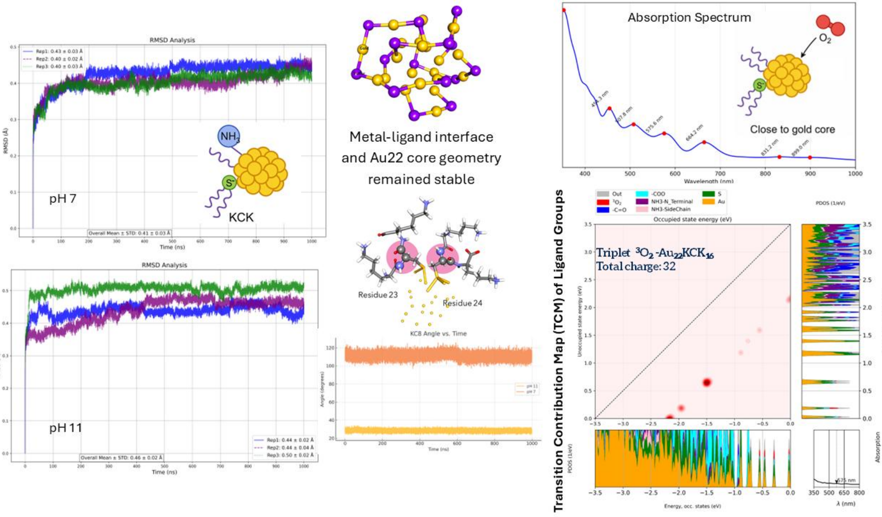


Figure 1: Conformational Dynamics (MD) and Electronic Excitations (DFT/TDDFT) of $Au_{22}(KCK)_{16}$ NCs

References

[1] P. Aminfar, T. Ferguson, E. Steele, E.M. MacNeil, M.F. Matus, S. Malola, H. Häkkinen, P.N. Duchesne, H. Loock, and K.G. Stamplecoskie, *Nanoscale* **16**, 205 (2024).

[2] H. Häkkinen, *Nat. Chem.* **4**, 443 (2012).

[3] C.M. Aikens, *J. Phys. Chem. Lett.* **2**, 99 (2011).

[4] R. Jin, *Nanoscale* **2**, 343 (2010).

[5] X. Kang and M. Zhu, *Chem. Soc. Rev.* **48**, 2422 (2019).

Poster 31

Compact Mach–Zehnder Interferometer Design for Improved Optomechanical Measurements in a Cryogenic Environment

Arash Mousavi Cheghabouri[1], Kalle Ihanus[2], and Juha Muhonen[1]

1- University of Jyväskylä, NanoScience Center, Hybrid Quantum Technologies in Silicon Group
2- University of Jyväskylä, Department of Physics

Realizing quantum-level measurement of optomechanical resonators requires high-stability optical interferometry to mitigate decoherence sources such as mechanical shaking. In our setup, the working of the cryogenic device introduced significant vibrational noise, limiting the fidelity of interferometric measurements. We report the development of a compact Mach–Zehnder interferometer with reduced spatial footprint and standardized equal beam height, overcoming limitations of our previous large-footprint design. To address cryostat-induced shaking, we implemented several stabilization measures, including leveling the optical table, lowering the breadboard, and rigidly fixing the breadboard to the table. These improvements resulted in enhanced mechanical stability and a marked increase in the quality of optomechanical measurements compared to our earlier configuration. Our results demonstrate that careful interferometer design and mechanical stabilization are essential steps toward achieving operations that pave the way for realizing precise optomechanical measurements of resonators.

Keywords: Mach-Zehnder Interferometer, Optomechanics, Mechanical Shaking

Poster 32

NbTiN-based superconducting refridgerators

Toivo Hakanen[1], Mika Prunnila[2] and Ilari Maasilta[1]
[1]Nanoscience Center, Department of Physics, P.O. Box 35, FI-40014 University of Jyväskylä, Finland
[2]VTT
Contact: toivo.a.hakanen@jyu.fi

As quantum computing and other applications of quantum physics become more prevalent, there is a growing need for alternatives to bulky and expensive cooling systems. On-chip solid-state coolers utilizing SINIS (Superconductor-Insulator-Normal conductor-Insulator-Superconductor) tunnel junctions could provide a complementary solution by providing local electronic cooling on-site, without the need to cool the entire substrate. These types of coolers can be easily controlled by adjusting the bias voltage across the junctions, and their operating range can be tuned by selecting different superconducting materials. The purpose of my research is to investigate methods for integrating NbTiN (highest superconducting critical temperature Tc of approximately 16 K) as a superconductor in SINIS coolers. The end goal is to engineer a high-Tc SINIS cooler, that could pave the way to cool down to sub-Kelvin temperatures from liquid He-4 bath.

Poster 33

Fabrication of quantum devices with focused helium ion beam

Aki Ruhtinas[1], Ilari Maasilta[1]
[1]*Nanoscience Center, Department of Physics, University of Jyväskylä, Jyväskylä, Finland*
Contact: akperuht@jyu.fi

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. 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. In addition to SQUIDs, we are currently investigating the use of directly written junctions for example in context of multiterminal Josephson junction devices.

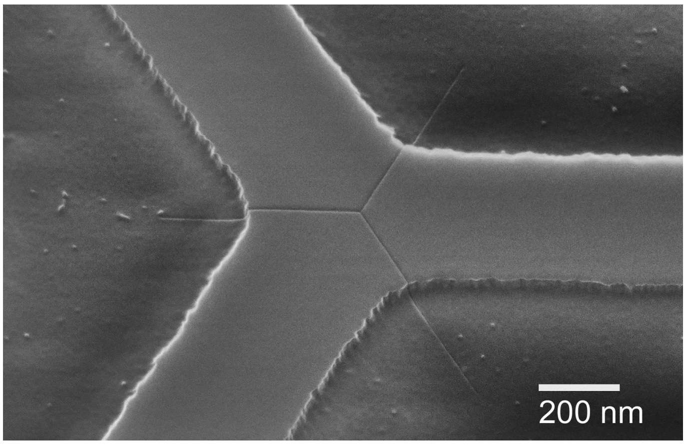


Figure 1: Helium ion microscope image of a three terminal Josephson junction formed with helium ion beam direct writing to a device made of 35 nm thick superconducting NbTiN film.

References

[1] S. Cybart et al., *Nat. Nanotechnol* **10**, 598–602 (2015)
[2] A. Ruhtinas and I. J. Maasilta, *arXiv:2303.17348* (2024)

Poster 34

Silicon optomechanical devices for spin coupling

Milla Männikkö, Henri Lyyra, Cliona Shakespeare, Simeoni Ahopelto, Kalle Ihanus and Juha Muhonen
Department of Physics and Nanoscience Center, University of Jyväskylä, P.O. Box 35, University of Jyväskylä FI-40014, Finland
Contact: mmmannik@jyu.fi

Quantum computation still lags behind classical computation in calculation speed due to the lack of scalable and noiseless architecture for multiple qubits. One avenue to achieve a quantum computer with minimal noise and a scalable number of qubits would be to use donor atom spins in silicon, as these have been shown to have a long coherence time[1]. The readout of such qubits would be implemented via optomechanics, which has multiple advantages, such as the fact that light is a lossless way to transport information and that it causes minimal disturbance on the measured object. The mechanics are a necessary bridge between the optics and the donor spin, but it can also be used to couple multiple of these qubits to each other. The spin-mechanical coupling can be achieved either via strain or micromagnets and the optomechanical coupling is achieved via the resonator, which is designed to be an optical cavity. As this spin mechanical coupling is yet to be observed, this poster will discuss a mechanical resonator with optimized design, its fabrication process and the coupling strength that this design achieves.

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`.

Poster 35

Temperature-controlled intermediates in the photocycle of the phytochrome from *Deinococcus radiodurans*

Roosa Vanhatalo[1], Dmitry Morozov[2], Heikki Takala[1], Gerrit Groenhof[2], Janne A. Ihalainen[1]
[1]*Department of Biological and Environmental science, University of Jyväskylä, P.O. Box 35, 40014 Jyväskylä, Finland*
[2]*Department of Chemistry, University of Jyväskylä, P.O. Box 35, 40014 Jyväskylä, Finland*

Contact: roosa.i.s.vanhatalo@jyu.fi

Bacterial phytochromes are red-light-sensitive photoreceptor proteins that enable organisms to respond to changing light environments. Photoactivation of these proteins begins with an absorption of a photon by the biliverdin IXα molecule, which is covalently bound to the protein. This absorption triggers an isomerization of the molecule, leading to protein scaffold changes and conversion between a red light-absorbing state (Pr) and a far-red light-absorbing state (Pfr). These states are thus distinguishable by their structures but also by their enzymatic activity. During the photoactivation from Pr state, the protein undergoes through Lumi-R and Meta-R intermediate states, until it reaches its photoactivated Pfr state. The photoactivation reaction has been characterized both in steady-state and kinetic experiments for the bacteriophytochrome from *Deinococcus radiodurans* [1-3]. We have revealed protein structures in their photostable Pr and Pfr states [1]. Furthermore, for the intermediate states, large-scale structural changes by means of X-ray scattering experiments and UV-Vis spectroscopic responses [2], as well as protein-chromophore interactions by means of IR-transitions [3], have been revealed. None of these experiments, however, directly probe the biliverdin helicity changes along the photocycle, which would rigorously test the recently proposed models obtained by the QM/MM simulations [4]. To address this, we aim to measure the circular dichroism (CD) spectra of these intermediates, for the first time.

Here, we present the cryogenic temperatures at which the highest population of the intermediates can be captured, as well as the UV-Vis spectra that reveal the intermediate states. We also show how Lumi-R forms in our CD measurements. We are working toward comparing the measured CD response of biliverdin in the intermediate states and the previous simulations, providing more ground for computational studies of the thermal protein scaffold relaxation processes during the photoactivation. Our approach reveals a direct comparison between computational and experimental results and enhances our understanding of chromophore orientation, dynamics, and behaviour during the photocycle. These insights will contribute to a mechanistic understanding of light sensing in bacteriophytochromes and deepen our ability to manipulate photoreceptor behaviour at the molecular level.

References

[1] H. Takala, et al., *Nature* **509**, 245 (2014).
[2] A. Björling, et al., *Sci. Adv.* **2**, e1600920 (2016).
[3] J.A. Ihalainen, et al., *J. Am. Chem. Soc.* **140**, 12396 (2018).
[4] D. Morozov, et al., *J. Phys. Chem. Lett.* **13**, 4538 (2022).

Poster 36

Enoyl-CoA-hydratase (ECH) catalyzed Enantioselective Hydration of 2E-Enoyl-SPAN *via* Simultaneous Activation of the Active Site Oxyanion Hole and Activation of H_2O molecule.

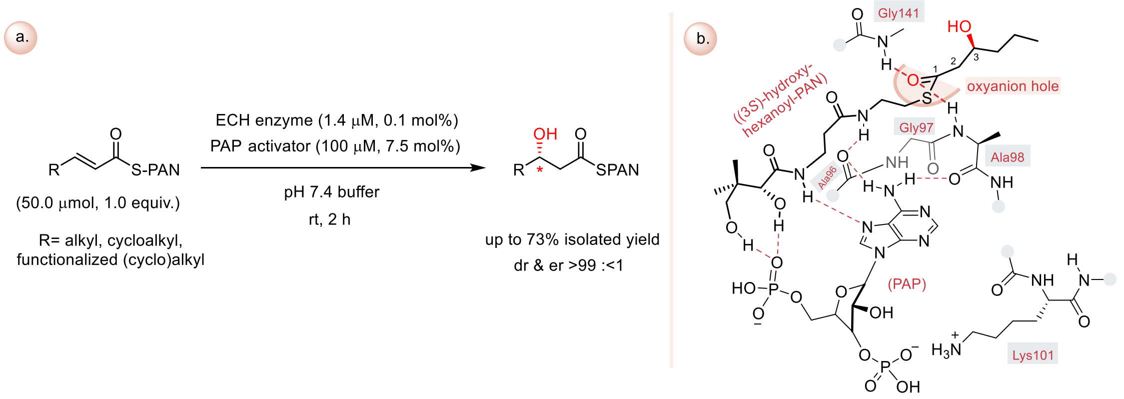
Subhadra Dalwani[1], Pradip Kumar Mondal[2], Werner Schmitz[3], Rik K. Wierenga[1] & Petri M. Pihko[2]

[1] Faculty of Biochemistry and Molecular Medicine, University of Oulu, P.O. Box 5400, FI-90014, Finland; [2]Department of Chemistry and Nanoscience Center, University of Jyväskylä, P.O.Box 35, FI-40014 JYU, Finland; [3]Theodor Boveri Institute of Biosciences (Biocenter), University of Würzburg, D-97074 Würzburg, Germany.

Contact: pkmondal@jyu.fi

Addition of water to α, β-unsaturated (thio)esters is synthetically a highly useful reaction, but currently synthetic catalysts to promote this transformation are lacking. Enzymes can promote this reaction with outstanding efficiency, as exemplified by the enzyme (2E)-enoyl-CoA hydratase (ECH), which catalyzes the addition of water to α, β-unsaturated thioesters. The drawback with ECH is that currently stoichiometric quantities of the expensive and hydrophilic CoA thioesters are required as substrates. We report herein a synthetic protocol for catalytic hydration with ECH, where CoA thioesters are replaced by more readily accessible pantetheine (PAN) thioesters. The key to success is that the catalytic activity of ECH is restored using an *activator*, 3',5'-ADP (PAP). ECH-catalyzed hydration of PAN thioesters with PAP co-catalyst proceeds rapidly at pH 7.4, under mild conditions, and with exceptional chemo- and near-perfect enantioselectivity, leaving potentially reactive functionalities in the substrate (such as primary halide, silyl ether or ester groups) completely intact.

We also provide structural insight into the activation of ECH by the PAP by X-ray crystallographic studies of ECH complexed with either the product derived from (2*E*)-enoyl-CoA or (2E)-enoyl-PAN + PAP. These structures show that PAP interacts with loop-2 of ECH and reconstitutes the oxyanion hole of ECH in a manner which is strikingly similar to the interaction of the native CoA with ECH.



Scheme 1: a. ECH catalyzed hydration reaction with (2*E*)-enoyl-PAN; b. Interactions of the (3*S*)-OH-C_6PAN thioester and PAP with the key active site residues of ECH (PDB ID: 9RGU).

References

[1] Waterson, R. M.; Hass, G. M.; Hill, R. L. *J. Biol. Chem.* **1972**, *247*, 5252–5257.
[2] Bahnson, B. J.; Anderson, V. E.; Petsko, G. A. *Biochemistry* **2002**, *41*, 2621-2629.
[3] Dalwani, S; Wierenga, R. K. *Current Opinion in Structural Biology* **2023**, *82*, 102671.
[4] Zhang, H.; Machutta, C. A.; Tonge, P. J. *In Comprehensive Natural Products II Chemistry and Biology* **2010**, *vol 8*, pp 231-275. Elsevier, Oxford, UK.
[5] Dalwani, S.; Mondal, P. K.; Schmitz, W.; Wierenga, R. K.; Pihko, P. M. *Manuscript under preparation*. PDB ID's for ECH liganded with (3*S*)-OH-C_6CoA: 9RGS and for unliganded ECH: 9RGQ.

Poster 37

Neural network acceleration of numerical simulation of methane combustion in a gas turbine engine

ANDRII CHEPURNYI, University of Latvia

Keywords: neural network, combustion, gas turbine engine, numerical simulation

Is demonstrated a practical route to faster, lower-cost design of low-emission gas-turbine combustors by pairing high-fidelity CFD with a compact neural-network surrogate. Trained on CFD data of methane combustion, a multilayer perceptron predicts NO_x and CO_2 with high accuracy (≈5–6% for NO_x; ≈1–2% for CO_2) across operating conditions defined by fuel flow, excess-air ratio, temperature, pressure, and cooling. The surrogate's outputs agree with experiments and a CRN model based on GRI-Mech 3.0, enabling rapid "what-if" exploration and optimization without rerunning full CFD. This capability supports digital-twin workflows and real-time combustion control, and the approach is readily transferable to alternative fuels (e.g., hydrogen, ammonia). Overall, the method accelerates emission assessment while preserving reliability, making advanced combustor design more agile and scalable.

Poster 38

Abstract

Intercalating magnetic Fe atoms into the layered van der Waals material TaS_2 produces an air-stable ferromagnet Ta_3FeS_6(1). The strong spin–orbit coupling of Ta atoms in the TaS_2 lattice, combined with the unquenched orbital angular momentum of Fe^{2+}, gives rise to hard ferromagnetism even in the two-dimensional limit. The resulting crystal exhibits high magnetic anisotropy, which stabilizes long-range ferromagnetic order and yields a remarkably large coercivity of 3 T. It is also a potential candidate for Kondo lattice due to the strong interaction of the localized magnetic moments and the itinerant conduction electrons(2). High SOC along with out of plane MCA results in topologically non trivial QSH states due to breaking of the time reversal symmetry. Large-scale images by scanning tunnelling Microsopy (STM) taken after cleaving the bulk crystal in ultrahigh vacuum reveal atomically flat terraces of the terminating S layer. The electronic properties investigated by tunnelling spectroscopy (STS) reveal a dip in the density of states close to the Fermi energy hinting a possible signature of Kondo lattice. Angle resolved photoemission studies also on the cleaved crystal also hint at some charge transfer into the host dz^2 conduction band.

References

1. Tianyou Zhai & Junbo Han et al, Adv. Mater. 2022, 34, 2107512(2014)
2. Yi Du & Wei Li et al, Nano Lett. 21, 6117 (2021)

Poster 39

Beyond Polariton Filtering: New Pathways for Polariton-Mediated Excitation

Ville Tiainen[1], Jussi Toppari[1]
[1]*Nanoscience Center and Department of Physics, University of Jyväskylä, Survontie 9, 40500, Finland*
Contact: ville.j.tiainen@jyu.fi

Strong light–matter coupling leads to the formation of polaritons—hybrid states combining molecular excitations with confined light. In Fabry–Pérot cavities, this requires sufficiently high molecular concentration, but higher concentrations also generate a dense manifold of dark states resonant with the molecular absorption. Excitations in such systems are delocalized and can transfer between bright polaritons and dark states depending on their spectral overlap [1]. Both simulations and experiments indicate that these states relax according to Kasha's rule, funnelling energy into the lowest available state [1–4].

Previously, we demonstrated that in strongly coupled 10-hydroxybenzo[h]-quinoline (HBQ), polaritons serve as gateways for transferring excitation into molecules, which then undergo excited-state intramolecular proton transfer similar to bare HBQ [5]. The efficiency of this transfer depends on the spectral overlap between polaritons and the molecular absorption.

Here, we further increase the coupling strength of the coupled HBQ system to reduce or eliminate this overlap. Under these conditions, excitation from the lower polariton is suppressed, while excitation from the upper polariton remains efficient—even when well above the molecular absorption band. This reveals additional energy transfer pathways beyond simple cavity filtering. Such mechanisms could extend the effective absorption range of molecules, with potential applications in enhanced light harvesting [3].

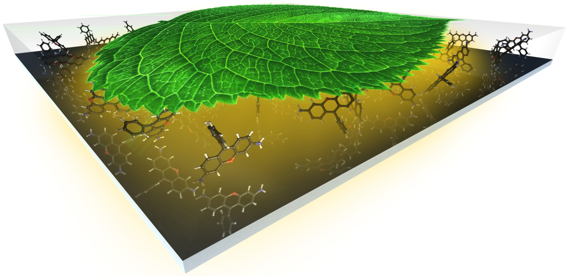


Figure 1: Artistic representation of polariton enhanced light-harvesting

References

[1] H.L. Luk, J. Feist, J.J. Toppari, G. Groenhof, J., *Multiscale Molecular Dynamics Simulations of Polaritonic Chemistry*, J. Chem. Theory Comput. 13 (2017).

[2] S. Baieva, O. Hakamaa, et al., *Dynamics of Strongly Coupled Modes between Surface Plasmon Polaritons and Photoactive Molecules: The Effect of the Stokes Shift*, ACS Phot. 4 (2016).

[3] G. Groenhof, J.J. Toppari, *Coherent Light Harvesting through Strong Coupling to Confined Light*, J. Phys. Chem. Lett. (2018).

[4] E. Hulkko, S. Pikker, V. Tiainen, et al., *Effect of molecular Stokes shift on polariton dynamics*, J. Chem. Phys. 154 (2021).

[5] A. Dutta, V. Tiainen, I. Sokolovskii, et al., *Thermal disorder prevents the suppression of ultra-fast photochemistry in the strong light-matter coupling regime*, Nature Commun. 15 (2024).

Poster 40

Beyond Eliashberg Theory of Superconductivity in flat-band systems

Natale Matranga[1], Tero T. Heikkilä [1], Risto Ojajärvi [1]
[1]*Department of Physics and Nanoscience Center, University of Jyväskylä, P.O. Box 35 (YFL), FI-40014 University of Jyväskylä, Finland*
Contact: natale.n.matranga@jyu.fi

Flat-band systems, with their nearly dispersionless electronic bands and high density of states, amplify interaction effects and challenge conventional theories of superconductivity [1]. Migdal-Eliashberg theory of superconductivity is based on the idea that electrons move much faster than the phonons, quantized vibrations of the atomic lattice, that mediate the pairing between them. Due to this separation of energy scales, certain interaction effects, called vertex corrections, can be neglected. This approximation, known as Migdal's theorem [2], has worked remarkably well in conventional superconductors [3]. However, in flat-band systems the conditions underpinning Migdal's argument no longer apply, and interaction effects that are usually negligible may start to matter. In this work, we investigate how vertex corrections influence superconductivity in flat-band systems, computing their leading contributions numerically, providing analytical estimates of their size, and examining how they affect the equation that governs the formation of superconducting pairs. Preliminary findings suggest that these corrections may play a significant role, highlighting the possible limitations of the standard Migdal-Eliashberg approach in flat-band superconductors and pointing toward the need for a more refined theoretical treatment in this unusual regime.

References

[1] Ojajärvi, Risto, et al. ”Competition of electron-phonon mediated superconductivity and Stoner magnetism on a flat band.” Physical Review B 98.5 (2018): 054515.

[2] Migdal, A. B. ”Interaction between electrons and lattice vibrations in a normal metal.” Sov. Phys. JETP 7.6 (1958): 996-1001.

[3] Allen, Ph B., and R. C. Dynes. ”Transition temperature of strong-coupled superconductors reanalyzed.” Physical Review B 12.3 (1975): 905.

Poster 41

Structural biology of infection and immunity

Sari Mattila[1] and Ilona Rissanen[1,2]
[1]*Institute of Biotechnology, HiLIFE, University of Helsinki, Viikinkaari 1, 00790 Helsinki, Finland*
[2]*Faculty of Biological and Environmental Sciences, University of Helsinki, Viikinkaari 9, 00790 Helsinki, Finland*
Contact: ilona.rissanen@helsinki.fi

Viruses are natural nanoscale assemblies, and studying their structures and dynamics not only reveals mechanisms of infection but also provides inspiration for nanoscience in areas such as self-assembly and drug delivery. The relatively simple composition of most viruses, together with the precise ways their proteins interact with cellular systems make them valuable model systems for exploring nanoscale principles in biology. Furthermore, understanding virus-host interactions is essential for devising effective strategies against infectious diseases. We apply X-ray crystallography, cryogenic electron microscopy, and protein engineering to investigate viral envelope glycoproteins that mediate host cell entry, and their interactions with neutralizing antibodies and cellular receptors. Here, we present highlights from our recent work, ranging from engineering antibodies to resolve neutralizing epitopes on pathogens such as the rabies virus [1], to the development of ultrapotent small proteins to neutralize SARS-CoV-2 [2,3], including a broadly cross-reactive small protein inhibitor that can neutralize all variants of concern by targeting a highly conserved site. Additionally, we examine conserved protein architectures regulating innate immune responses and metabolism to uncover novel targets for therapeutic intervention. This integrative approach provides insights into viral protein functions and immune targeting, advancing both fundamental virology and the design of innovative antiviral strategies.

References

[1] Kedari A et al. Structural insight into rabies virus neutralization revealed by an engineered antibody scaffold. *Structure*. **32**:2220-2230. (2024).
[2] Hannula L et al. Nanobody engineering for SARS-CoV-2 neutralization and detection. *Microbiology Spectrum* **12**: p. e0419922. (2024).
[3] Mäkelä AR et al. Intranasal trimeric sherpabody inhibits SARS-CoV-2 including recent immunoevasive Omicron subvariants. *Nature Communications* **14**: p. 1637. (2023).

Poster 42

Controlling Phosphorescence of Bisphosphonium Salts

Eetu Hakkarainen[1], Andrei Beliaev[1], Igor O. Koshevoy[1]
[1]*Department of Chemistry and Sustainable Technology, University of Eastern Finland, Yliopistokatu 7, 80100 and Joensuu, Finland*
Contact: eetu.hakkarainen@uef.fi

Phosphorescent molecular materials attract constant attention as their utilization spreads across various high-end technologies such as sensors, displays, bioimaging, and phototherapy.[1] Developing efficient, easy-to-synthesize, and eco-friendly luminophores is necessary, as these technologies should follow a net zero-emission objective of the EU directive by 2050.[2] In this regard, phosphonium species, which are composed of organic π-conjugated cations and inorganic anions, can become superior candidates due to two main reasons. First, their rigid, solid-state ionic structure blocks non-radiative transitions, resulting in increased efficiency. Secondly, the structures of both constituents can be easily modified to give rise to tunable optical properties. Importantly, the anions can be altered from simple halides or their inorganic counterparts, increasing the number of heavy atoms.[3] This allows for modulating the intersystem crossing rate, potentially increasing the ability to harvest triplet excitons more efficiently.

As the optical properties of such ionic luminophores arise from the interplay of the two constituents, we have designed and tested a series of ionic pairs **1**–**4** consisting of a naphthalene-based bisphosphonium cation and different heavy counterions, including halides (Br^- or I^-) and a set of metallates (CdI_4^{2-}, $ZnBr_4^{2-}$). In the solid state, these species exhibit high quantum yields, reaching 75% for **1** and fast radiative rates of up to 2.14×10^5 s^{-1} for **3**. The lifetimes of the excited state vary from 1.3 μs to 2.4 ms, while the emission maxima span from 542 nm to 568 nm (Figure 1).

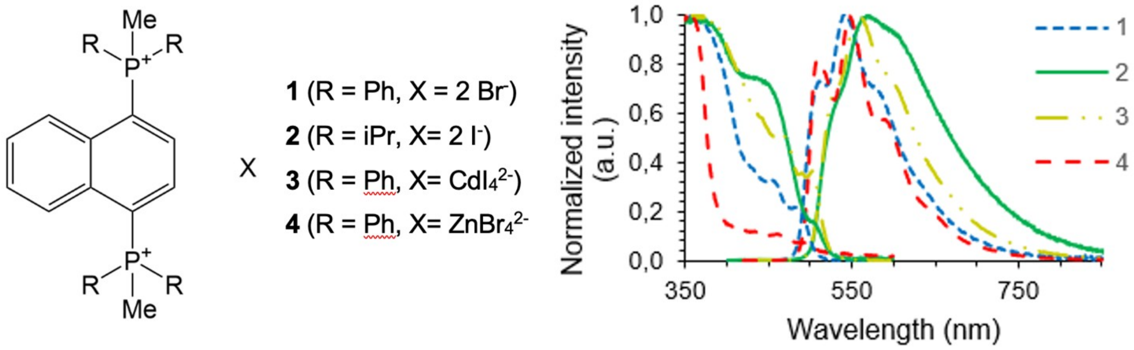


Figure 1: Structures of the studied salts (left) and their emission profiles (right).

References

[1] Franca, L. G., et.al. *ACS Appl. Opt. Mater*. **2024**, 10.1021/acsaom.4c00041.

[2] European Commission, Directorate-General for Climate Action, Publications Office **2019**, doi/10.2834/02074.

[3] Dai, W., et.al. *Chem. Sci.* **2024**, 15 (12), 4222–4237.

Poster 43

The water droplet contact line probed with multiwalled carbon nanotubes at the air-water interface

Esa Hyyryläinen, Juha Merikoski, Markus Ahlskog
Department of Physics and Nanoscience Center, University of Jyvaskyla, FI-40014, Finland
Contact: markus.e.ahlskog@jyu.fi

The coffee ring effect involves the drying behavior at the contact line of droplets of colloidal dispersions. Functionalized carbon nanotubes, that are modestly dispersible in water, have also been explored as the colloidal particles [1]. As such, their extremely high aspect ratio is of interest to probe the intricate behavior of the contact line. Pristine carbon nanotubes are hydrophobic and thus non dispersible in water. We used a special technique that distributed hydrophobic multiwalled carbon nanotube (MWNT) material on the surface of a spreading and eventually drying water droplet [2]. We observed end-to-end ordering of the MWNTs into chain-like structures, that are particularly prominent next to the triple phase contact line of the sessile droplet (Fig.1). Capillary interactions among the MWNTs at the air-water interface, is seen to be the driving force for the ordering [3]. These MWNT chains are also useful for probing the contact line motion of evaporating water droplets. We have two theoretical approaches to describe the experimental observations. The first one is to consider the energetics of the system as the MWNTs interact with the gas-liquid interface, in particular close to the contact line. This we do at the level of van der Waals interactions. The observations can in part be understood as a consequence of capillary interactions. Our second approach is to study the contact line and interface folding. This is caused by contact line pinning due to MWNTs and graphitic impurity particles and leads to local changes in the interface curvature driving capillary interactions [4].

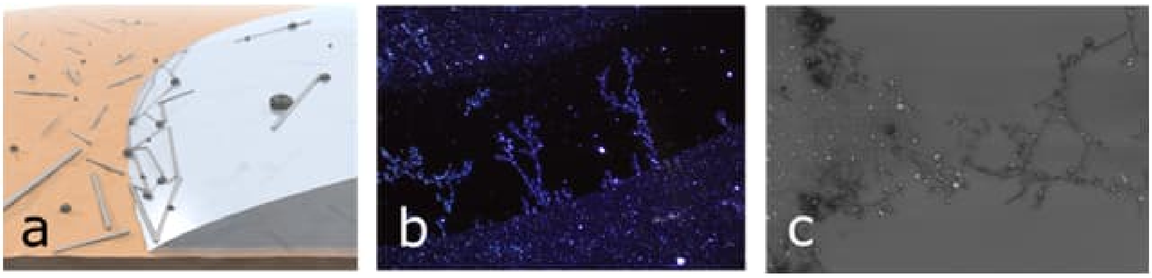


Figure 1. (a) Illustration of MWNTs lifted up on water droplet (b) Optical microscope image of capillary ordered MWNT chains at the perimeter of the droplet imprint, after the droplet has completely dried. (c) A close-up SEM view of the starting point of the chains. Here graphitic impurity particles attached to the tubes are visible.

References

[1] H. Li, TC Hain, A Muzha, F Schöppler, T Hertel, *ACS Nano*, **8**, 6417 (2014).
[2] MJ Hokkanen, S Lautala, E Flahaut, M Ahlskog, *Colloids and Surfaces A*, **533**, 109 (2017).
[3] IB Liu, N Sharifi-Mood, KJ Stebe, *Ann. Rev. of Cond. Matt. Physics*, **9**, 283 (2018).
[4] E. Hyyryläinen, J. Merikoski, M. Ahlskog, Under review.

Poster 44

A new technique based on multiwalled carbon nanotubes for exploring early phase spreading of water droplets

Kasperi Paloniemi, Juha Merikoski, Markus Ahlskog
Department of Physics and Nanoscience Center, University of Jyvaskyla, FI-40014, Finland
Contact: markus.e.ahlskog@jyu.fi

The very early phase of the dynamic spreading process of liquid droplets (usually water) is an ongoing topic of study. There are different configurations, among which the joining and merger of two droplets is one widely studied case, while another, and the theme of this work, is the spreading of a droplet on a smooth substrate. The latter involves the serious problem of the behavior of the triple phase contact line. As was very recently reviewed in ref. [1], there are still numerous open questions on this topic.

In the case of spreading over a smooth surface, one may conceive as an experimental technique having the surface covered by mobile nano- or micron-sized particles, eg. carbon nanotubes [2]. With a monolayer of unconnected such particles, conceivably the spreading droplet can create a pattern/imprint within it and yield such experimental information of spreading processes, that are difficult to obtain via other means. Here we present results on this kind of experiments.

Figure 1. Left: High speed camera data of a sessile water droplet brought into contact with a silicon chip carrying a 2D deposit of multiwalled carbon nanotube (MWNT) material. Right: Optical micrograph of resulting imprint in the MWNT deposit.

References

[1] J Eggers, JE Sprittles, JH Snoeijer, **57**, 61 (2025).
[2] MJ Hokkanen, S Lautala, E Flahaut, M Ahlskog, *Colloids and Surfaces A*, **533**, 109 (2017).