

NANOSCIENCE DAYS 2026

ABSTRACT BOOK



NSC
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UNIVERSITY OF JYVÄSKYLÄ

Unless specifically mentioned, the program will take place in **Sokos Hotel Alexandra**, Ihantola room.

Monday 5.10.2026

08.30–09.30	Registration, Main lobby	
08.30–09.30	Coffee + visit the sponsors	
09.30–09.45	Opening words, Dean Timo Sajavaara	
09.45–10.45	Plenary I	Frauke Gräter
10.45–11.45	Plenary II	Sergio Padilla-Parra
11.45–12.00	LaboLine Oy	
12.00–13.30	LUNCH BREAK + visit the sponsors	
13.30–14.30	Plenary III	Bruno Frka-Petesic
14.30–15.15	Coffee + visit the sponsors	
15.15–16.30	Plenary IV	Kari Rissanen
16.30–18.00	Poster session with refreshments, restaurant Frans & Sandra	
18.00	University of Jyväskylä campus tour	
19.30	Conference Dinner	
20.00	Keräilyerät - Band	

Tuesday 6.10.2026

09.00–09.45	Coffee	
09.45–10.45	Plenary V	Sarah Haigh
10.45–11.45	Plenary VI	Adrian Bunzel
11.45	Merck Life Science, Discovery, Advanced and Process Solutions	
12.00–13.00	LUNCH BREAK + visit the sponsors	
13.00–14.00	Plenary VII	Jovana Milic
14.00–15.00	Plenary VIII	Johanna Ivaska
15.00–	Closing ceremony, Head of NSC Fabien Cougnon	

Plenary speakers

1. **Frauke Gräter**
Mechanoradicals in living matter: how mechanical forces generate oxidative signals
2. **Sergio Padilla-Parra**
Integrative imaging to understand HIV-1 Env conformational dynamics
3. **Bruno Frka-Petesic**
Cellulose nanocrystal self-assembly into nanostructured photonic materials
4. **Kari Rissanen**
Intermolecular interactions in action
5. **Sarah Haigh**
Probing dynamic atomic behaviour at surfaces and interfaces
6. **Adrian Bunzel**
Creating enzymes by computational design and directed evolution
7. **Jovana Milic**
Supramolecular control in hybrid perovskite materials: from photovoltaics to neuromorphics for sustainable energy technologies
8. **Johanna Ivaska**
Integrin mediated cell adhesion in modulation of cancer progression

Mechanoradicals in living matter: how mechanical forces generate oxidative signals

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Tissues are perpetually subjected to mechanical forces. We know for nearly a century that high mechanical load on polymer materials - be it a shoe sole or rubber band - causes the rupture of chemical bonds and generates mechanoradicals. We uncovered the very same mechanism in biology: radicals form by stretching collagen and elastin, major proteins material of our tissues, even under stresses far below tissue failure. Using experiments in conjunction with simulations and machine learning, we reveal how the extracellular matrix tames its radicals and converts them in a highly controlled fashion to oxidative stress, dominantly hydrogen peroxide. We currently explore how this new mechano-sensing mechanism is related to disease and ageing.

Plenary II

Integrative imaging to understand HIV-1 Env conformational dynamics

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HIV-1 maturation is essential for viral entry, yet linking Gag processing to Env organization and structure has remained challenging. Here, we combine a newly developed intraviral FRET biosensor, DNA-PAINT and cryo-electron tomography to establish this relationship at the single-virus level. The FRET biosensor, genetically packaged into HIV-1 particles and validated under both room-temperature and cryogenic conditions, quantitatively identifies fully immature, partially mature and mature virions. This enables what we term functional CLEM, where fluorescence lifetime microscopy provides quantitative functional information in cryogenic conditions. Correlating maturation state with Env organization, we show that early Gag cleavage promotes Env clustering and stabilizes the metastable closed State 1 conformation, whereas immature particles display dispersed Env in a partially open state. Furthermore, CLEM - CryoET confirms distinct Env architectures in immature and mature particles. Beyond revealing how maturation controls Env dynamics, this work establishes functional CLEM as a new paradigm in which light microscopy delivers quantitative molecular information rather than simple contrast.

Cellulose nanocrystal self-assembly into nanostructured photonic materials

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Cellulose nanocrystals (CNCs) are anisotropic and chiral colloidal nanorods that can be extracted from various cellulosic bio-sources and represent a promising building block for the development of renewable and multifunctional nanomaterials. Remarkably, CNCs can spontaneously form a colloidal liquid crystal above a threshold volume fraction, with a left-handed cholesteric order, and upon further solvent evaporation can produce nanostructured films that display strong spectral reflection in the visible range, resulting in vivid structural colour.¹⁻³

In this talk, I will discuss various aspects of the mechanisms responsible for such effect and explore the various routes to control and utilise this phenomenon, from elucidating and controlling the chirality of CNCs at the individual level, to the implementation of strategies and constraints to drive their self-assembly into various nanostructured architectures, such as external fields, confinement or buckling instabilities.

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Intermolecular interactions in action

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An exciting research challenge in supramolecular chemistry is to design, synthesize, and characterize nano-sized architectures with applications in biology, chemistry, and materials science.¹ Predicting and designing non-covalently bound supramolecular complexes and assemblies is difficult because of the weakness of the interactions involved, thus the resulting superstructure is often a compromise between the geometrical constraints of the building blocks and the competing weak intermolecular interactions.² Our research over 30 years has been focused on the studies of weak non-covalent intermolecular, viz. supramolecular interactions as the driving force in self-assembly and molecular recognition, especially in the solid state by single crystal X-ray diffraction. The lecture will highlight some of our studies on halogen-bonded,³ especially halogen(I) systems, anion... π ⁴ interactions and metal ion coordination⁵ in molecular self-assembly and molecular recognition.

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Probing dynamic atomic behaviour at surfaces and interfaces

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Scanning Transmission Electron Microscopy (STEM) enables direct imaging of local atomic structure and elemental composition to uncover structure-property relationships. For example, we have used this to uncover local nanostructure and thus support development of improved performance in ferroelectric films¹ and in electrocatalysts for water oxidation catalysts.² Yet (S)TEM imaging is typically performed in high vacuum environments which can cause artefacts relative to the sample in operando conditions. In situ (S)TEM using specialist holders or instruments enables imaging under more realistic environmental conditions. In this talk I will present some of our recent work illustrating how we have used STEM liquid cells to probe growth of tellurium nanowires, informing strategies for bulk electrodeposition at lower potential.³ I will also report how we have applied in-situ gas cell STEM to investigate how the catalyst morphology evolves during activation heat treatment of cobalt oxides depending on the amount of doping with Mn promotor to optimise performance of Fischer Tropsch catalysts.⁴ I will also report experiments using our graphene heterostructure liquid cells, which allow atomic resolution spatial resolution of solid catalysts surrounded by liquids including atomic scale dynamics at a solid-liquid interfaces.⁵ We have developed a new polymer-free transfer technique to produce such graphene cells with minimal contamination and for a wide range of solvents.⁶ Here we will report how this approach can be combined with an automated Noise2void machine learning image analysis pipeline⁷ to allow new investigations of the dynamic behaviour of 10000-1000000 individual atomic sites at solid-liquid interfaces as a function of solvent environment.⁸

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Creating enzymes by computational design and directed evolution

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Deep learning is revolutionizing protein design and structure prediction, enabling us to engineer biology with unprecedented accuracy. Enzymes are nature's molecular machines that carry out chemistry with atomic precision. Computational design now lets us not only create entirely new enzymes, but also organize proteins on the nanoscale to enhance their reactivity. In our group, we combine computational protein design with directed evolution¹⁻³ to create new-to-nature enzymes for solar-energy conversion.⁴

To advance computational enzyme design, we recently developed Al.zymes,⁵ an integrative platform that combines deep learning-based protein design and structure prediction tools to systematically optimize enzyme activity, selectivity, and stability. We validated Al.zymes by designing an enzyme from scratch that accelerates a C–H bond cleavage reaction by a millionfold over the uncatalyzed reaction. Building on this framework, we computationally designed light-harvesting protein nanowires, nanoscale structures that bind photosensitizers and electron transfer cofactors to drive light-induced electron transfer.⁴ These nanowires are applied in biohybrid solar cells to convert sunlight into electricity. To further improve their performance, we submitted the nanowires to directed evolution. In iterative rounds of mutagenesis and screening, we improved their photovoltaic efficiency by nearly an order of magnitude. Currently, we are harnessing self-assembly to organize these nanowires into two-dimensional sheets that densely coat electrode surfaces with a nanolayer of photoenzymes. Ultimately, our work addresses critical sustainability challenges, enabling biocatalysts for not only photovoltaics but also solar-powered carbon capture and nitrogen fixation.

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Supramolecular control in hybrid perovskite materials: from photovoltaics to neuromorphics for sustainable energy technologies

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Hybrid organic-inorganic framework materials have emerged as one of the most promising semiconductors in optoelectronics.¹ In particular, hybrid halide perovskite materials have demonstrated superior solar-to-electric energy conversion in photovoltaics. These are soft yet crystalline mixed ionic-electronic semiconductors with remarkable optoelectronic characteristics.^{2,3} However, their limited stability in response to environmental factors, such as oxygen and moisture, as well as under operating conditions of voltage bias and light, hamper practical applications.⁴ This is the result of ion migration that contributes to the reactivity at the interface, limiting stability under device operating conditions.² There has been an effort to overcome these shortcomings by developing tailored organic components that template hybrid perovskite frameworks and contribute to their stabilization through increased hydrophobicity and limited ion permeability, enhancing their performance in optoelectronics.^{5,6} We demonstrate the capacity to rely on supramolecular engineering to develop a new generation of hybrid perovskite materials that respond to external stimuli and adapt to their operating conditions, such as by incorporating photochromic systems into ‘smart solar cells’ that can adapt to day-night cycles.⁷ The dynamic control of the underlying ionic migration has set the basis for the utility of these materials in brain-inspired memory elements, as artificial synapses,⁸ and self-powered memories for neuromorphic computing,⁹ revealing new perspectives for hybrid framework materials, and more sustainable lead-free systems,¹⁰ in emerging technologies.

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Integrin mediated cell adhesion in modulation of cancer progression

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Tissue homeostasis is dependent on the spatially controlled localization of specific cell types and the correct composition of the extracellular stroma. Integrins are the main cell adhesion receptors of extracellular matrix (ECM) ligands. They integrate ECM cues to the cellular cytoskeleton and regulate key cellular signalling pathways. By nucleating new adhesion sites and regulating the turnover of existing adhesions, integrins and components of the actin cytoskeleton control cell morphology, polarity and migration. In all adherent cell types, integrins are essential regulators of tissue homeostasis and their mis-regulation is implicated in several diseases, including cancer and inflammation. Integrin-mediated adhesions, in conjunction with the actin cytoskeleton, regulate cell fate and identity and allow cells to migrate and invade the surrounding ECM.

Tight control over integrin mediated adhesion and signalling is paramount for normal cell function and is perturbed in almost every step of cancer progression. Our long-standing interest is in uncovering cancer relevant integrin-associated proteins and signalling networks. We have used RNAi screens to identify new proteins implicated in the regulation of integrin activity, integrin traffic, cell migration and metastasis. We are continuing this work by 1) investigating in mechanistic detail adhesion regulating protein networks using proximal-biotinylation, by 2) developing FRET-based probes to map the spatiotemporal regulation of integrin signalling under different conditions, by 3) screening for cell response to varying ECM compositions and 4) by exploration of integrins in mechanosensing and mechanotransduction.

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POSTER ABSTRACTS



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Watching Dyes Bind: FLUPS Reveals the Interaction Pathways of Ethidium Bromide and SYBR Green with Carbon Dots

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Carbon dot (CD)-based fluorescent sensors depend on dye-nanomaterial interactions that control signal generation, sensitivity, and selectivity, yet their ultrafast mechanisms remain poorly understood. In our previous work, we developed an ultrasensitive ratiometric enteroviral RNA sensor based on enhanced electron transfer from CDs to ethidium bromide (EB), achieved through covalent functionalization of CDs with short oligonucleotide probes (CDs-Probe/EB; Figure 1a,b).[1] The functionalized sensor enabled direct viral RNA detection with a sensitivity range of 0.3-5 nM and a limit of detection (LOD) of 67 pM, substantially outperforming non-functionalized sensors.

Here, we investigate the excited-state processes underlying this enhanced response using femtosecond fluorescence upconversion spectroscopy (FLUPS; Figure 1c). FLUPS resolves CD-EB electron transfer dynamics with sub-picosecond resolution, allowing extraction of transfer time constants and identification of competing relaxation pathways responsible for CD quenching and EB signal enhancement. Femtosecond transient absorption spectroscopy further confirms non-radiative relaxation channels and dye-specific excited-state behavior.

We also extend this approach to SYBR Green, a widely used and less hazardous nucleic-acid dye, to compare its interaction and electron-transfer mechanism with CDs against that of EB. By linking ultrafast kinetics to ratiometric sensing performance, this study provides a mechanistic basis for rational dye selection in CD-based sensors. The results demonstrate how controlled electron-transfer pathways govern sensor sensitivity and establish FLUPS as a powerful tool for guiding the design of next-generation, amplification-free viral RNA detection platforms.[2,3]

Acknowledgements. This work was supported by the Nanoscience center, JYU, project no. 21002180, and by the Research Council of Finland through the Academy of Finland consortium project “HARVEST” (project no. 2100006383).

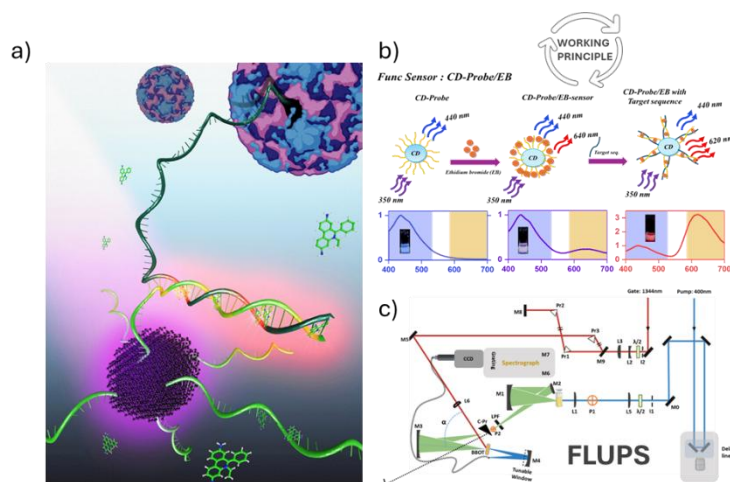


Figure 1. (a) Schematic of CDs-dye-nucleic acid interactions enabling binding-induced fluorescence modulation. (b) Ratiometric sensing mechanism based on electron transfer from CDs to ethidium bromide upon target binding, leading to CDs quenching and EB emission enhancement. (c) Femtosecond fluorescence upconversion spectroscopy (FLUPS) setup used to resolve ultrafast electron transfer dynamics between CDs and intercalating dyes.

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Bismuth Oxychloride-Polyethylenimine Nanoparticles for Computed Tomography Contrast-Enhanced Cartilage Imaging

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Background: Early osteoarthritis (OA) is characterized by subtle compositional changes in articular cartilage, particularly loss of anionic proteoglycans (PGs), which cannot be detected in the clinic with conventional medical imaging.[1] Contrast-enhanced computed tomography (CT) offers a quantitative approach for probing cartilage microscopic composition.[2,3] However, currently available molecular contrast agents (CAs) are not optimal for cartilage imaging because of limited cartilage uptake and insufficient X-ray attenuation, creating a need for novel CAs that combine these features. We hypothesize that bismuth oxychloride-polyethylenimine nanoparticles (BiOCl-PEI-NPs), as an ultrasmall cationic CA, interact with the PGs of cartilage and can therefore be used for CT-based cartilage imaging and evaluation of cartilage health (Fig.1.a) **Methods:** BiOCl-PEI-NPs were synthesized by hydrolysis of bismuth(III) chloride followed by two-step coating process, and the resulting NPs were characterized. *Ex vivo* bovine osteochondral plugs ($d = 7$ mm) from medial femoral condyle were assigned to healthy, early OA, or late OA groups ($n = 1$), with OA induced by trypsin ($c = 0.5$ mg/mL, 37°C) for 1 or 16 h, respectively, followed by immersion in CA ($c_{\text{NP}} = 80$ mg/mL). Samples were imaged in air by μCT at 0, 2, 6, 23, 47, 72, and 90 h of NP immersion, followed by PBS washout. **Results:** FTIR, zeta potential, and TEM analyses supported successful formation and PEI functionalization of the NPs. The BiOCl core had an average diameter of 3.5 ± 0.6 nm and therefore is small enough to penetrate the dense cartilage matrix, which has a pore size of ~ 6 nm.[4] The zeta potential shifted from -15.9 ± 1.4 mV for the uncoated BiOCl core to $+4.9 \pm 0.6$ mV after PEI coating. The BiOCl-PEI-NP CA exhibited an X-ray attenuation of 326 ± 30 Hounsfield Units (HU). NP diffusion into cartilage was associated with tissue health: healthy cartilage exceeded 500 HU whereas late OA cartilage 300 HU (Fig.1.b). After PBS washout the NPs were completely removed from all samples (Fig.1.c). **Conclusions:** BiOCl-PEI-NPs provided strong CT contrast in cartilage with healthy, early OA, and late OA samples showing differences in NP uptake and diffusion behavior. The combination of higher uptake into healthier cartilage and complete washout suggests that these ultrasmall NPs can offer a solution for contrast-enhanced CT evaluation of cartilage composition, while avoiding the persistent tissue retention observed with non-clearing cationic agents.[5]

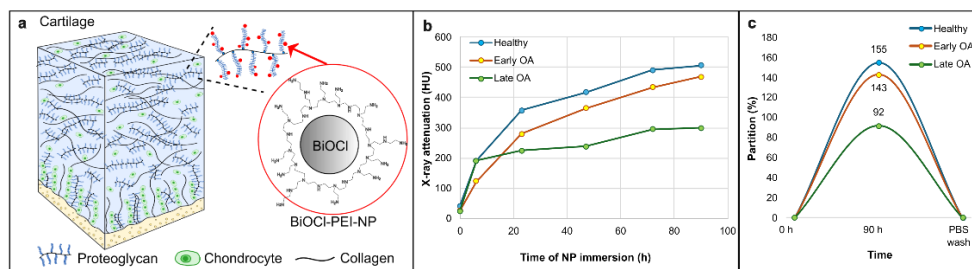


Figure 1. (a) Schematic illustration of BiOCl-PEI-NP and its interaction with cartilage proteoglycans. (b) Bulk X-ray attenuation values of healthy, early OA, and late OA cartilage groups at different time points during NP immersion. (c) Contrast agent partition values of the three cartilage groups before NP immersion, at 90 h, and after PBS washout.

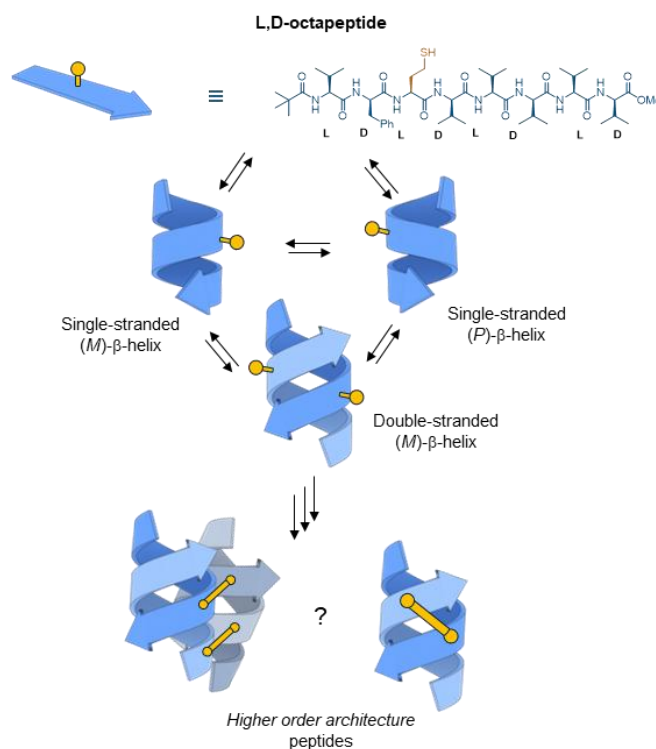
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Structural Analysis of β -Helical Stapled Heterochiral Peptides

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Expanding protein structure beyond the canonical motifs found in nature remains a central challenge in *de novo* design.¹⁻⁴ Heterochiral amino acid sequences offer a potential route to access unconventional architectures exhibiting conformational states that are inaccessible to homochiral sequences.⁵⁻⁶ In particular, valine-based heterochiral octapeptides form in chloroform complex libraries of unusual helical structures, including single β -helices (right- and left-handed) and double β -helices. Our group is currently investigating whether the introduction of cysteine residues can provide access to higher-order architecture *via* the formation of disulfide bridges between strands. This work aims at establishing heterochiral peptides as versatile building blocks for constructing higher-order, noncanonical protein-like architectures.



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Pulsed laser deposition of high-quality superconducting epitaxial NbTiN thin films for quantum devices

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We report the fabrication of high-quality superconducting NbTiN thin films on MgO (100), C-plane Sapphire (0001) and amorphous SiN substrates by using the reactive pulsed laser deposition (PLD) technique. The thickest NbTiN thin films exhibit magnificent superconducting properties, with high critical temperature (T_c) of about 16 K and low normal state resistivity (ρ_n) $\sim 35 \mu\Omega\text{cm}$ at 20 K. Moreover, no significant influence of the substrates on the T_c is observed. However, the substrates play an influential role on the resistivity (ρ_n) of NbTiN films and lower ρ_n is observed for MgO substrate. Interestingly, the thinnest (~ 4 nm) ultrathin NbTiN films demonstrate a T_c of about 7.3 K and the resistivity ($\rho_n^{20\text{K}}$) $\sim 93 \mu\Omega\text{cm}$ on MgO substrate. Further, the compositional analyses as performed by using elastic recoil detection analysis (ERDA) and Rutherford backscattering spectroscopy (RBS) reveal low impurity concentrations and relatively little variations in the ratio of (Nb+Ti)/N which was close to unity in most of the films. Besides, from the structural characterization by using x-ray diffraction (XRD) technique, the NbTiN films grown on MgO and sapphire substrates are observed as highly crystalline in cubic (FCC) structure with lattice orientations (2 0 0) and (1 1 1), respectively. However, on SiN substrate, films were not strongly oriented but maintained a similar range of T_c . Finally, high-quality NbTiN thin films fabricated by PLD technique can be used for superconducting quantum devices such as helium-ion beam defined Josephson junctions [1], superconducting qubits, kinetic inductors, single photon detectors (SNPDs), etc.

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Optical Properties of Metal-Ion-Mediated Au₂₅ Nanocluster-Based Assemblies

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Building cluster-assemblies from superatomic building blocks, where each cluster behaves as an elemental atom, has attracted interest in the past decades due to their enhanced optical properties. Herein, we study the optical properties of recently discovered gold nanocluster assemblies mediated by Mg(II), Co(II), Ni(II) and Cu(II) metal ions [1] using time-dependent density functional theory (TDDFT). Depending on the coordinating metal ion, the assemblies exhibited different absorption spectra with a redshift of up to 51 nm. Surprisingly, our calculations revealed that the assemblies have chiroptical response, despite being assembled from achiral building blocks [2]. The chirality emerges from the coordination complex formed between the coordinating metal ions and the carboxylic acid groups of the ligands, and is transferred to the achiral nanoclusters. These theoretical findings may influence experiments to create enantioselective nanocluster assemblies.

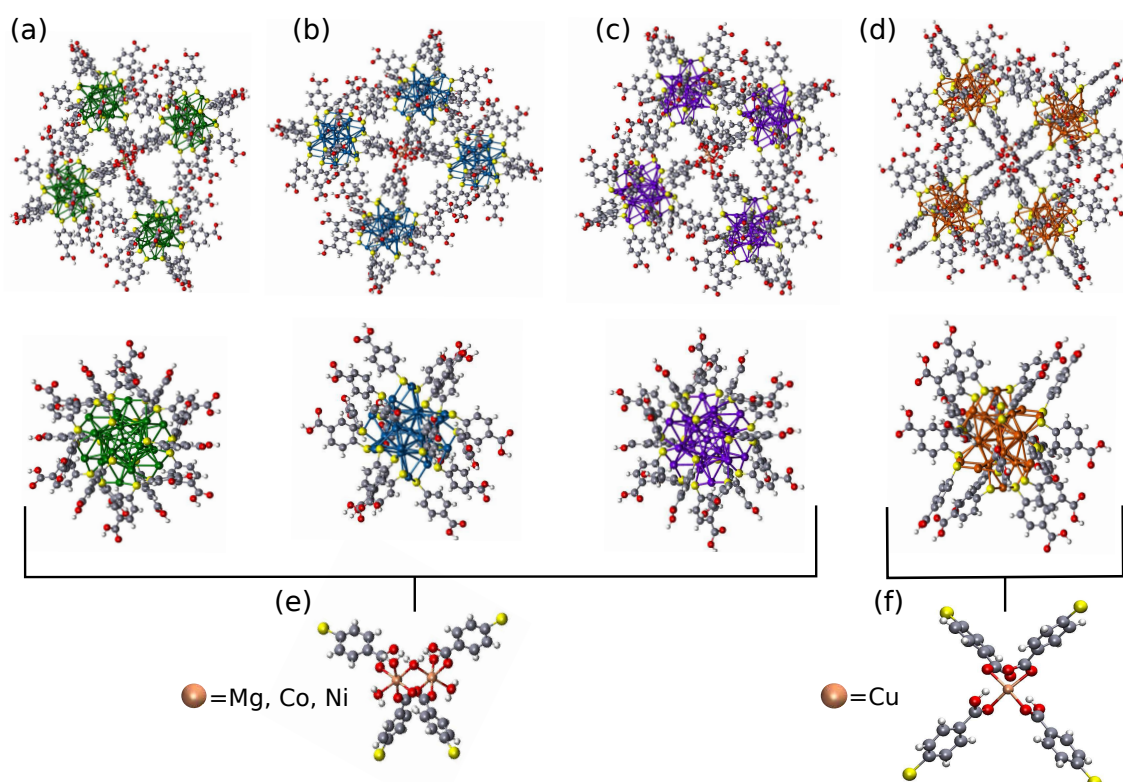


Figure 1: Structures of (a) Mg, (b) Co, (c) Ni, and (d) Cu mediated $[\text{Au}_{25}(\text{p-MBA})_{18}]^{-}$ assemblies, together with their isolated $[\text{Au}_{25}(\text{p-MBA})_{18}]^{-}$ cluster, represented in green, blue, violet, and orange, respectively. (e) The connecting node for (a)–(c), and (f) the connecting node for (d). C, O, H and S atoms are shown in gray, red, white, and yellow, respectively.

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Building-Block Assembly Controls ON/OFF Luminescence in Isomeric Au₇Cu₈ Nanoclusters

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Two isomeric Au₇Cu₈ nanoclusters, assembled from identical Au₄Cu₃ pentagonal-bipyramidal building blocks but with different connectivity, exhibit strikingly different photophysical behavior: Au₇Cu₈-1 is strongly phosphorescent, whereas Au₇Cu₈-2 is essentially non-emissive. This pronounced contrast, despite their closely related compositions and building units, raises an important question regarding how the assembly mode controls the electronic and excited-state properties of the clusters. To shed light on the origin of this behavior, we performed density functional theory and excited-state calculations to investigate their electronic structures, optical absorption, spin–orbit coupling, and competing relaxation pathways.

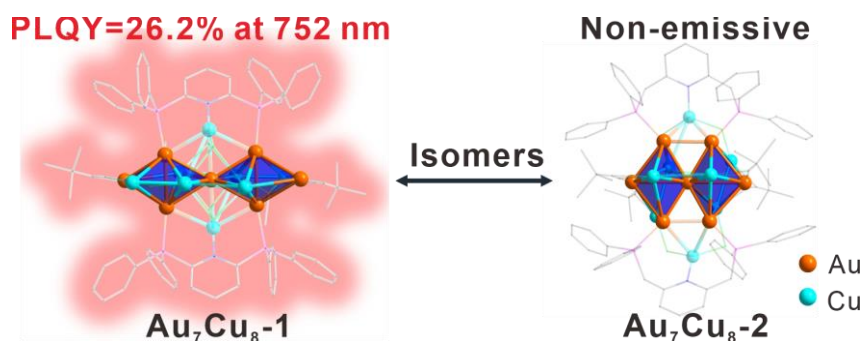


Figure 1: Contrasting photophysical behavior of isomeric Au₇Cu₈ nanoclusters: Au₇Cu₈-1 is strongly phosphorescent (PLQY = 26.2%, λ_{em} = 752 nm), whereas Au₇Cu₈-2 is essentially non-emissive.

Computational X-ray Absorption Spectroscopy of Gold Nanoclusters

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Gold nanoclusters (NCs) are tiny molecules with a gold core protected by an organic ligand layer. They possess a wide range of applications, facilitated by their designability at the atomistic level [1]. They are used e.g. to destroy antibiotics resistant superbacteria[2], purify water[3] or in medicine as biosensors[4]. X-ray absorption spectroscopy (XAS) can provide information about orbital specific density of states, oxidation states, core electron binding energies and the bonding types occurring in molecules and nanoclusters. Interpreting this data at a single atom level needs a detailed and trustful approach to simulate the XAS properties of NCs atom by atom. Here, we investigate L-edge X-ray absorption near edge spectroscopy (XANES) for reference bulk systems and the carbene protected Au₁₃ NC[5] and interpret details of latter's electronic structure. We show that XAS properties of gold atoms inside the cluster are very diverse depending on their chemical environment and symmetry. Our work deepens the understanding of spatial variations of local oxidation states, charge distributions, and chemical bonding environments of gold atoms inside ligand-protected clusters, highlighting the impact of diverse ligand environments.

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Photoisomerizable peptide-based supramolecular gelators

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Supramolecular peptide-based gels with tunable, photoresponsive properties represent a promising class of adaptive soft materials. Peptide-based systems are of particular interest due to their structural diversity, inherent biocompatibility and strong gelation capability. [1,2] These gels form through the self-assembly of low molecular weight gelators (LMWGs) driven by weak, non-covalent interactions, including hydrogen bonding, π - π interactions and hydrophobic effects. Incorporation of photoresponsive units into the gelator framework enables remote control of gel structure and material properties using light as an external stimulus. [3] Stilbene and azobenzene are representative photoactive moieties that undergo reversible *cis-trans* isomerization upon ultraviolet irradiation, enabling photoinduced conformational changes in gelator molecules that may trigger transitions between gel and solution states (Figure 1). [4] Here, the synthesis of potential stilbene- and azobenzene functionalized peptide gelators is presented. The synthesized compounds serve as a platform for investigating photoinduced effects on gelation behaviour.

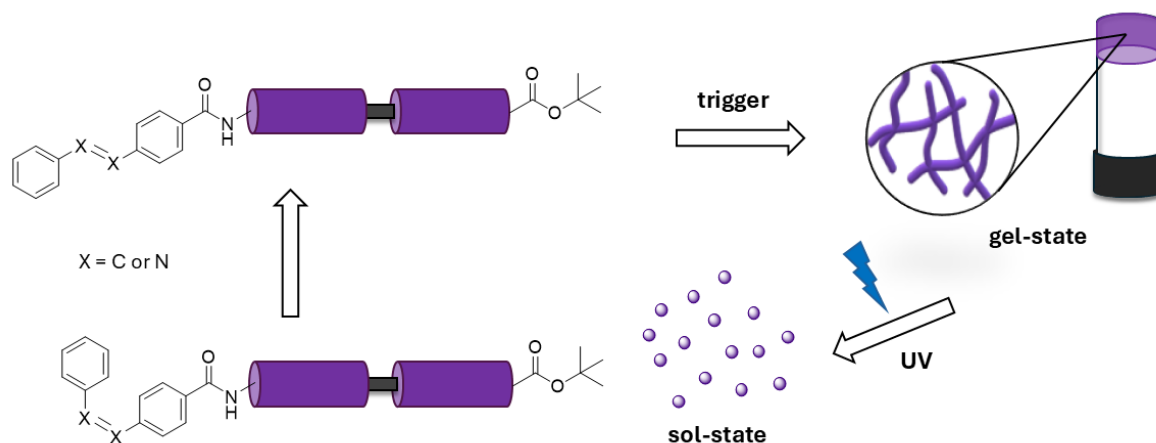


Figure 1. Schematic presentation of gel formation and photoinduced gel-to-sol phase transition of photoisomerizable peptide-based gelators. Purple blocks represent amino acids.

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Exploring boreal freshwater jumbophages: from isolate diversity to transcriptional regulation

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Jumbobacteriophages encode unusually large genomes and complex infection machineries, yet their infection-stage transcriptional programmes remain poorly characterised, particularly in non-model environmental hosts. Here, we compared two genomically distinct jumbophages, FKo-1 (385,083 bp) and FKo-2 (230,309 bp), that infect the same *Flavobacterium* sp. host, allowing for phage-specific infection strategies to be studied in a shared host background. First, infection dynamics were characterised using host growth and culture-lysis experiments. Early, middle and late transcriptomes were profiled by ONT-cappable-seq at 30, 90 and 180 min post-infection for FKo-1 and at 30, 60 and 110 min for FKo-2, with the sampling points selected to represent equivalent infection stage. Transcription-boundary signals were mapped, and coding DNA sequence (CDS) expression was classified as temporally specific when the peak CPM was at least 10 and at least twofold higher than at the second-highest stage. Both phages showed slow infection cycles, but FKo-1 was delayed relative to FKo-2: free phage titres began to increase after approximately 180 and 100 min, respectively, with apparent burst sizes of approximately 90 and 120 PFU per infected cell. FKo-1 also displayed a more sharply partitioned transcriptional programme. In total, 453/583 CDSs (77.7%) were temporally specific in FKo-1, compared with 176/312 (56.4%) in FKo-2. Expression was regionally coordinated across both genomes. FKo-1 contained an extensive origin-spanning early block, an early NAD-associated island, a middle-enriched sigma-factor region and a late structural-gene region. FKo-2 contained an early-biased host-interface island whose expression remained prominent at the middle stage. Thus, even in a shared host background, these jumbophages differed substantially in both replication timing and the temporal organisation of gene expression. The larger, slower FKo-1 showed stronger temporal partitioning, highlighting long-read, boundary-aware transcriptomics as a powerful approach for resolving the complex infection programmes of jumbophages.

Fabrication of Ordered SiN Pillar-based PnCs with Integrated Heater and Thermometer to Study Thermal Transport Mechanism in Coherent Regime

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Fabricating a periodic structural design to control the propagation and dispersion of phonons has offered a prominent platform to engineer thermal transport at the nanoscale. These structures are referred to as Phononic Crystals (PnCs). Manipulating the lattice periodicity and feature size of these PnCs to correspond to the dominant thermal phonon wavelengths gives rise to various wave-mechanical phenomena such as the emergence of phononic bandgaps [1] and flattening of the bands that reduce the in-plane thermal conductivity dramatically. Here we present the fabrication and preliminary electrical characterization of pillar-based PnCs fabricated on a suspended silicon nitride (SiN) membrane. Utilizing multiple steps of e-beam lithography and reactive ion etching, a two-dimensional array of micron-scale SiN pillars has been realized on a low-stress SiN membrane. The thermal measurements are facilitated by integrating a Superconductor-Normal metal-Superconductor (SNS) micro-heater and a Superconductor-Insulator-Normal metal-Insulator-Superconductor (SINIS) thermometers [2] that are positioned at the center of the PnC region. Here we report on the preliminary quality check of the integrated SNS and SINIS sensors as the full thermal transport measurements are currently in progress. The integrity of the metallic contact pads with the SNS heater is confirmed by the room temperature electrical characterization. Furthermore, the SINIS tunnel junctions exhibit high-quality IV-characteristics with characteristic large superconducting gaps and minimal sub-gap leakage when measured at sub-Kelvin temperatures in an Adiabatic Demagnetization Refrigerator (ADR). These junctions can therefore be used as robust thermometers suitable for high-sensitivity thermal sensing. The future outlook of this research will thus be to quantify the effects of phononic crystals on low-temperature heat flow in the coherent regime.

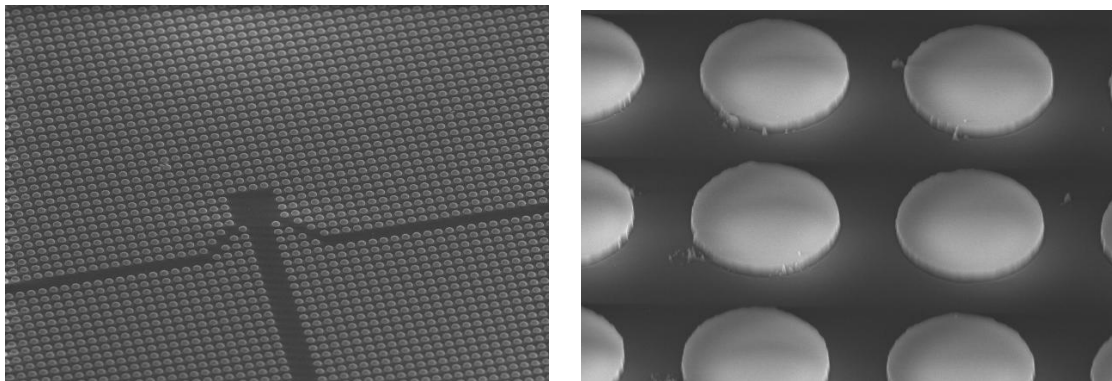


Figure 1: Ordered SiN Pillar-based PnCs

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The first cultivated megaphage bridges metagenomic dark matter and cellular life

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The discovery of megaphages has extended the known size limits of bacteriophages far beyond expectations. Their enormous genomes appear counterintuitive for a host-dependent lifestyle and raise fundamental questions: are megaphages evolutionary outliers, or do large genomes provide adaptive advantages? Phages with genomes exceeding 600 kbp were initially discovered through metagenomic data [1]. In silico approaches provide valuable insights into viral diversity, yet the functional biology of these unique phages remains largely unexplored due to the lack of isolates. In our laboratory, we investigate cultivable megaphages from boreal freshwater ecosystems that infect *Flavobacterium* strains. The first isolated representative, FKy-1, is a myovirus with a ~160 nm icosahedral head and a ~180 nm tail. Its 646,765 bp genome is predicted to encode 1,068 CDSs, 68 tRNAs, 6 tmRNAs, and diverse auxiliary metabolic genes. The presence of an expanded set of transcription- and translation-related genes, including ribosomal protein genes, suggests a complex phage–host interaction strategy. Here, we present the first transcriptomic dataset for a megaphage across the infection cycle. We characterize the temporal structure of the FKy-1 transcriptional program and provide a basis for investigating the adaptive strategies of huge phages.

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Emitted power from double quantum dot and hexagonal lattices nanojunctions

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We study electroluminescence, the light emission as a consequence of current through nanojunction, through the profile of emitted power. In particular, we focus on the following nanojunction as quantum emitter: a double quantum dot. The model is analyzed for future applications to a hexagonal lattice (a model for a benzene molecule), which can also be extended to periodic structures such as graphene nanoribbons. Non-equilibrium Green's function formalism [1] is used to study the electronic behavior while a classical approach is applied to the radiation field [2]. Using the time-dependent Landauer-Büttiker formalism [3], which follows from exact analytical solutions to the Kadanoff-Baym equations describing the molecular junction subject to an arbitrary time-dependent bias, we then determine the photon self-energy and the associated emitted power [2].

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NbTiN-based superconducting refrigerators

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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 our research is to investigate methods for integrating NbTiN (highest superconducting critical temperature T_c of 15.7 K [1] achieved in house) as a superconductor in SINIS coolers. Characterization of NbTiN-NbTiNOx-Au and NbTiN-NbTiNOx-Cu junctions show that it is possible to reach a low reduced Dynes parameter of 10^{-3} , which is below the upper limit of 10^{-2} to achieve any cooling at all, see Figure 1. The end goal is to engineer a high- T_c SINIS cooler, that could pave the way to cool down to sub-Kelvin temperatures from over 1 K [2], ideally from a liquid He-4 bath.

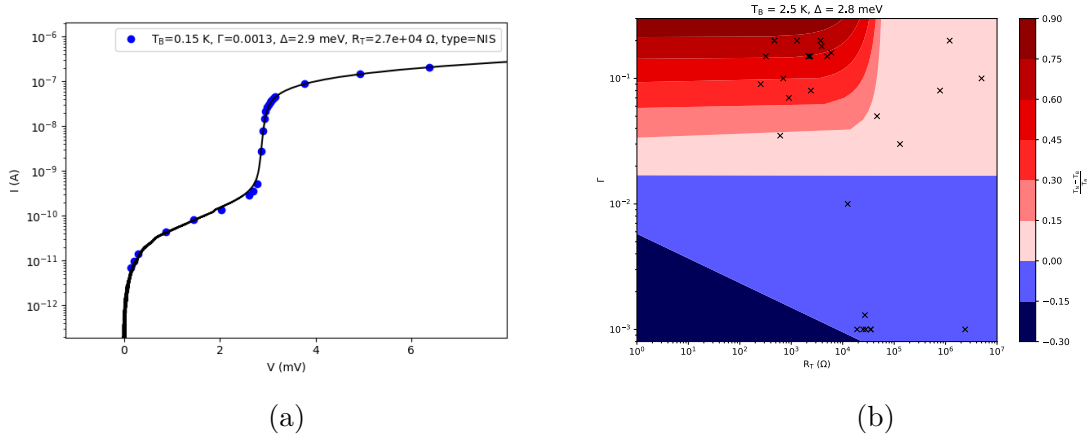


Figure 1: A sub-kelvin transport measurement of a single NIS-device in 1(a) and a collection of characterized devices on a Dynes - R_T plot in 1(b). Color map in 1(b) corresponds to lowest relative temperature difference between Normal metal and bath in 1(b), which are calculated using optimal bias voltage [3] and typical device dimensions. T_B is the bath temperature (also the superconductor temperature), T_N is the normal metal temperature, R_T is the tunneling resistance of a single junction, Δ is the superconducting gap at 0 K and Γ is the reduced Dynes parameter.

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Material-Efficient Electrospray Deposition of Polydopamine Films with Tunable Morphology

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Polydopamine (PDA) is a bio-inspired polymer capable of forming adherent coatings on a wide range of materials. However, conventional solution-based deposition provides limited control over thin-film formation and typically consumes considerably more material than is incorporated into the coating. Here, we combine stable aqueous PDA stock solutions produced by heterogeneous Cu(0)-assisted dopamine oxidation [1] with electrospray deposition (ESD) to obtain controlled PDA thin films.

Electrospray deposition converts the PDA solution into charged microdroplets whose evaporation and interaction with the substrate determine the resulting film structure. By controlling the deposition conditions, we obtain reproducible PDA coatings with tunable thickness and surface morphology. The transition between different morphologies is consistent with changes in the extent of solvent evaporation before droplet impact, providing a route to control PDA film formation through the electrospray process. In addition, ESD substantially increases material utilization compared with conventional solution-based PDA coating methods [2].

The combination of controllable PDA synthesis and electrospray deposition (Fig. 1) therefore provides a material-efficient route to nanostructured PDA films and establishes relationships between droplet-scale processing conditions and nanoscale coating morphology.

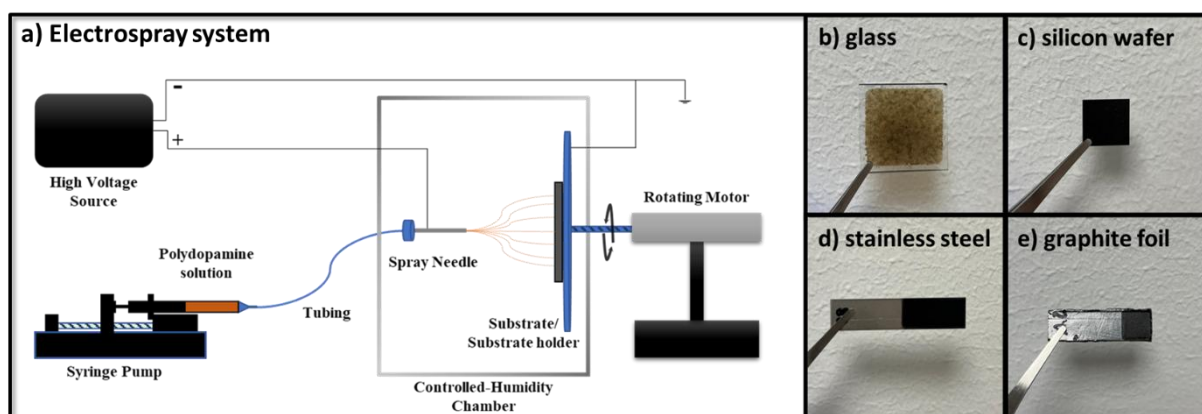


Figure 1. (a) A scheme of the electrospray deposition apparatus, (b-e) electrospayed PDA coatings on different substrates.

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Accelerating Atomic Configuration Identification on Reconstructed Surfaces with Machine Learning

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Surfaces of solid-state materials play a crucial role in many technological applications, such as heterogeneous catalysis connected with production of green fuels or preparation of semiconductor devices. However, on the nanoscale the atomic surface structure of many materials are still unknown, even in the simplest case of surfaces in vacuum, leaving a huge knowledge gap of physics and chemistry of surfaces. In the past the computational search for the atomic structure of surfaces has been driven by chemical intuition or ab-initio molecular dynamics. But the recent developments in machine learning (ML) allows for going beyond the limits of computational approaches.

In this work, I am presenting my ML aided workflow (Fig. 1) for predicting the atomic structure of surfaces, mainly for semiconductors and oxides: Starting from automatized tool for passivation of bottom side to reinforcement learning based tool able to build few top layers of (reconstructed) surface, enhancing the original strategy by [1]. To speed-up and computationally cheapen the workflow, I will be employing already pre-trained ML interatomic potentials, like MACE-MP [2]. Simultaneously, I will be complementing to development of the pre-trained (universal) potential to be better working on reconstructed surfaces.

Through this tool, I aim to seal the knowledge gap and therefore contribute to development of new semiconductor devices or heterogeneous catalysts for cheaper production of green fuels.

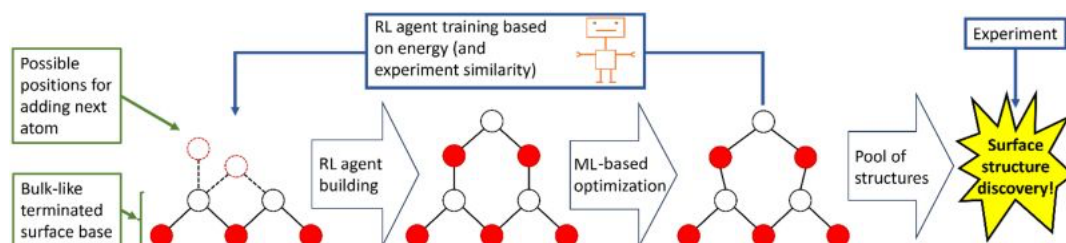


Figure 1: The automatized workflow is using building final layer(s) of the surface reconstruction using Monte Carlo sampling (MC) or reinforcement learning (RL) agent for placing atoms to the new layer. Fine-tuned MLIP, like MACE-MP, will be used for intermediate optimizations and final energy estimation for training of the RL agent and selection of candidates. The most promising once will be then calculated on full density functional theory level followed by experiment simulations. These will be then compared with the actual experiments.

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Red light-sensing optogenetic tool for breast cancer treatment

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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 [2,3].

Breast cancer is the most common cancer worldwide in women and has still several subtypes without effective treatment. To address this, we will harness our far-red light-activatable tool mFREDusk to induce production of pro-apoptotic proteins, and hence apoptosis. The tool will be delivered to breast cancer 3D models using viral vectors. We are currently optimizing our apoptosis-inducing system across different cell lines, with the aim of inducing apoptosis in “hard to cure” cancers such as triple negative breast cancer. Once successful, our optogenetic apoptosis-inducing system could provide a non-invasive alternative to currently available cancer therapies.

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Effect of water on cellulose crystallization: insights from hydrogen bonding by molecular modeling

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The plant cell wall is a complex composite material, and its nanoscale structure plays an important role in determining the mechanical properties and functionality of plants. Cellulose microfibrils are a major structural component of the cell wall, and their crystallization plays a significant role in the formation of the cell wall. However, the molecular mechanisms of cellulose microfibril formation, particularly the influence of the surrounding environment and intermolecular interactions, remain poorly understood. In this work, we conduct molecular dynamics simulations based on the known structure of the plant cellulose synthase complex (rosette^[1]) and investigate the formation behavior of cellulose microfibrils in vacuum and aqueous systems. By comparing the structural evolution of cellulose in vacuum and hydrated environments, we aim to understand how the presence of water affects the crystallization process. We analyze hydrogen-bonding interactions within and between cellulose chains to investigate how differences in hydrogen bonding relate to the distinct aggregation behavior observed in the two systems. These results provide molecular-level insights into the environmental dependence of cellulose microfibril formation and the role of hydrogen bonding in this process. This contributes to a better understanding of cellulose organization in plant cell walls and provide a molecular basis for interpreting experimental observations.

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Area-Selective Atomic Layer Deposition of Metals on Laser-Oxidized Graphene

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Polymer residues generated during conventional lithographic fabrication remain a critical bottleneck limiting the performance of graphene-based electronic devices [1]. Area-Selective Atomic Layer Deposition (AS-ALD) offers a scalable lithography-free route to deposit materials precisely on graphene while preserving its intrinsic properties.

Our approach combines femtosecond laser-induced two-photon oxidation (2PO) of graphene with metal deposition by ALD. The 2PO process promotes the incorporation of oxygen-containing groups (hydroxyl and epoxy) into the graphene lattice at submicrometer resolution (300 nm) [2]. Thanks to this functionalization, AS-ALD on oxidized graphene areas can be achieved [3], where differences in surface reactivity promote precursor nucleation and growth. Using this platform, we investigate AS-ALD of gold (Au), a key material for graphene-based devices, leveraging recently developed reductive Au ALD chemistry [4]. By systematically varying laser parameters, we precisely tuned the degree of oxidation and correlated it with subsequent Au nucleation and growth behavior under different ALD conditions.

Results show a clear dependence of Au growth on 2PO degree, switching from selectivity to antiselectivity at medium oxidation levels. Low-degree 2PO areas exhibit an increased Au island density compared to pristine graphene, demonstrating partially selective growth (Fig. 1). Conversely, at high-degree 2PO areas, this behavior reverses, and Au growth is suppressed, leading to antiselective deposition. In addition, graphene has been proved to be compatible with the employed Au ALD reaction, opening a new path to deposit Au nanoparticles on pristine graphene in a controllable and reproducible way.

These findings demonstrate that 2PO enables systematic control over ALD behavior on graphene and provides a route toward contamination-free, spatially defined metallization. In search of better selectivity for deposition, critical for device applications, our ongoing work has extended this approach to palladium (Pd) AS-ALD. First experiments have shown excellent selectivity.

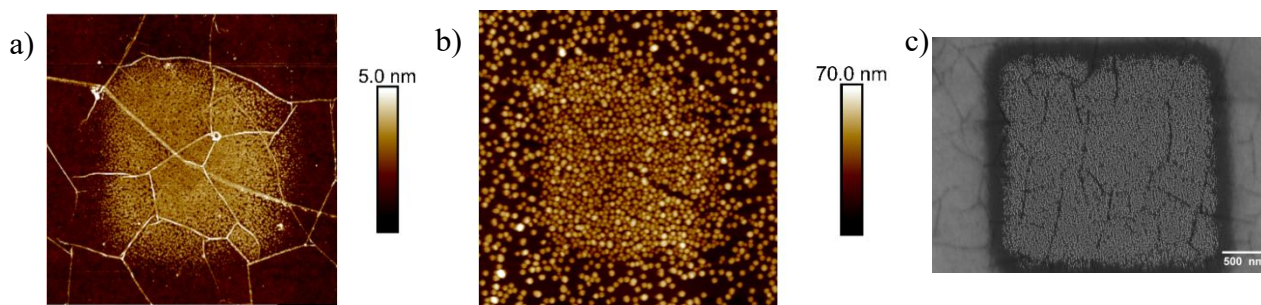


Figure 1: AFM topography images of graphene a) after low-dose 2PO b) after Au ALD. Scale bar is 670 nm. C) SEM image of 2PO graphene after Pd ALD.

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Improvement of the Simmons model for tunnel junctions

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We present an improvement [1] of the so-called Simmons model [2-5], which is a well-known, extremely highly cited (Ref. [3] has more than 3800 citations, for example) and still widely used analytical model to calculate the tunneling current (or conductance) of tunnel junctions, established already in the 1960s. It can be used, for example, to estimate the most critical material parameters of the tunneling barrier, such as its thickness and height in energy, from simple electrical measurements.

Such an improvement is relevant for modern science, as tunnel junctions are used more and more in applications in quantum technology, such as building blocks of superconducting qubits, superconducting quantum interference devices (SQUIDs), sensitive radiation detectors, on-chip electronic coolers and thermometers. In the quest to explore more advanced barrier materials and fabrication methods for those applications, the old theoretical models [2-5] reach their limits of applicability, and more accurate models need to be developed, with a wider range of applicability for different barrier types.

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Dynamic electrostatic mosaic in the ligand layer of water-soluble $\text{Au}_{25}(\text{p-MBA})_{18}$ nanocluster

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Water-soluble monolayer-protected gold nanoclusters (AuNCs) are atomically precise nanomaterials with molecule-like properties that make them attractive for applications ranging from catalysis to biomedicine. Their hybrid structure enables precise engineering of physical properties, solubility and functionality. In aqueous environments, ligand-ligand and ligand-environment interactions are strongly influenced by ligand charge distributions, which are governed by pH but remain incompletely understood. A molecular-level understanding of ligand deprotonation is therefore essential for the rational design of AuNC reactivity, solvation and application-specific functionality.

To investigate the effect of pH, we employed the constant-pH molecular dynamics method [1] for statistical sampling of ligand charge distributions in a water-soluble gold nanocluster protected by *para*-mercaptobenzoic acid ligands, $\text{Au}_{25}(\text{p-MBA})_{18}$, in a wide pH range of 1 to 11. The results revealed three macroscopic pK_{a} values for the ligand layer: 2.25 ± 0.01 , 5.68 ± 0.02 , and 6.23 ± 0.04 , and indicated anticooperative deprotonation behavior with Hill coefficients ranging from 0.74 to 0.34. The ligand layer arrangement and interligand interactions through π - π stacking explained the observed deprotonation sequence. These results uncover ligand-specific deprotonation behavior of $\text{Au}_{25}(\text{p-MBA})_{18}$, providing molecular-level insight for the rational design of AuNCs in diverse applications including catalysis, biosensing platforms, drug delivery systems, and pH-responsive materials.

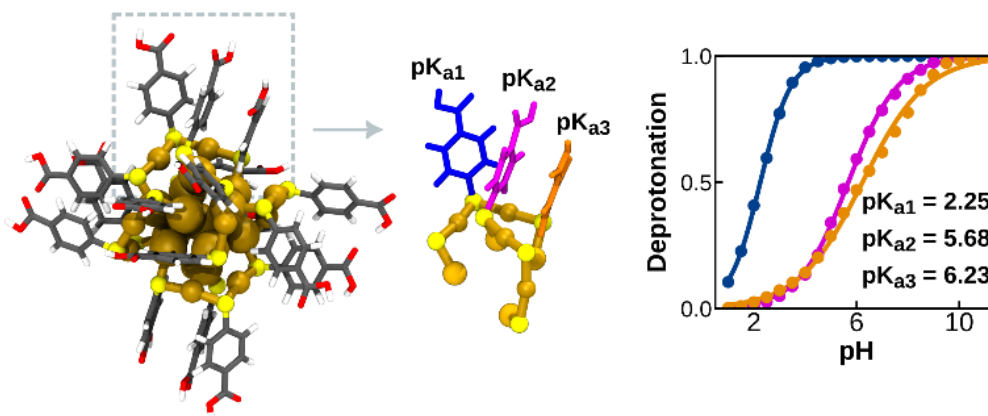


Figure 1: Ligand-shell organization and interligand π - π stacking correlates with the three-step deprotonation behavior of $\text{Au}_{25}(\text{p-MBA})_{18}$.

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Loading Efficiency of Apigenin, Luteolin and Bromelain onto Metal Oxide-Based Nanomaterials

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Metal oxide-based nanomaterials are promising platforms for the immobilization and delivery of biologically active compounds due to their physicochemical stability and tunable surface properties [1-3]. The aim of this study was to evaluate the loading efficiency of selected bioactive compounds differing in their chemical nature onto functionalized metal oxide-based nanomaterials. Apigenin and luteolin, representing flavonoids, and bromelain, a proteolytic enzyme, were selected as model bioactive compounds. Nanomaterials based on ZnO, CeO₂, Ga₂O₃, Bi₂O₃ and Gd₂O₃ were investigated. To modify their surface properties and obtain multicomponent carrier systems, selected formulations additionally contained antioxidant components and surface coatings. Different combinations and amounts of these additives were investigated to assess their potential influence on bioactive compound loading.

Loading efficiency was determined indirectly based on the concentration of the unbound compound remaining in the supernatant after the loading procedure. The obtained results revealed a clear compound-dependent behavior. Both flavonoids showed consistently high affinity toward the investigated metal oxide-based materials. Apigenin loading efficiencies generally exceeded 94%. Similarly, luteolin showed high loading efficiencies, predominantly above 95%. In contrast, bromelain exhibited substantially greater variability depending on the composition of the nanomaterial. For selected CeO₂-based systems, considerable bromelain loading was observed, whereas considerably lower apparent loading was obtained for some other oxide-based formulations. The results indicate that not only the type of metal oxide but also the presence and composition of additional antioxidant and coating components may contribute to differences in loading behavior.

Overall, the findings demonstrate the potential of multicomponent metal oxide-based nanomaterials as platforms for the immobilization of structurally diverse bioactive compounds and provide a basis for further optimization of their composition for bioactive compound delivery.

Keywords: metal oxide nanomaterials; bioactive compounds; flavonoids; loading efficiency

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A Modular Approach to the Functionalization of Metal Oxide Nanoparticles with Bioactive Molecules

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The development of multifunctional nanomaterials requires flexible strategies that enable the combination of inorganic nanostructures with bioactive molecules exhibiting different physicochemical and biological properties. In this study, a modular approach to the surface functionalization of metal oxide nanoparticles was investigated. The designed systems were based on ZnO, CeO₂, Ga₂O₃, Bi₂O₃ and Gd₂O₃ as inorganic cores and were sequentially modified with selected antioxidants, bioactive compounds and surface-coating molecules.

The proposed strategy involved three functionalization levels. In the first step, metal oxide nanoparticles were modified with selected antioxidants, including tannic acid, ascorbic acid, retinol and tocopherol. Subsequently, apigenin, luteolin or bromelain was introduced as the bioactive component. In the final functionalization step, selected formulations were additionally coated with glutathione, mannose or galactose. Different combinations and amounts of individual components were investigated to evaluate the versatility of the proposed modular design and the possibility of tailoring the composition of the resulting nanomaterials.

The obtained results confirmed that the developed approach enables the preparation of a broad range of multicomponent metal oxide-based systems. The efficiency of bioactive compound incorporation depended on both the chemical nature of the loaded molecule and the composition of the carrier. Particularly high loading efficiencies were observed for the flavonoids apigenin and luteolin across different formulations, while bromelain showed more composition-dependent behavior. The results also indicate that the selection of the metal oxide core and additional surface modifiers provides multiple possibilities for controlling the final composition and properties of the nanomaterials.

Keywords: multifunctional nanomaterials; metal oxide nanoparticles; surface functionalization; bioactive compounds;

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Free-Energy-Guided Prediction of Gold Nanocluster Binding Sites on Blood Proteins

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Gold nanoclusters (AuNCs) are atomically precise nanoparticles with tunable ligand-shell chemistry. Atomistic understanding of their interactions with biomolecules would facilitate their rational design for biomedical applications. While Molecular dynamics (MD) simulations provide atomistic resolution, their effective use is hindered by the lack of starting structures: experimental structures of bound complexes are unavailable, and conventional docking approaches remain unreliable due to complexity of AuNCs. Unbiased MD simulations can reveal dynamically accessible binding sites, but sampling is computationally expensive. Simultaneously, these simulations generate rich datasets that could be leveraged to develop predictive models for binding-site identification in related systems. Previous predictive models based on interaction energies often produce unstable predictions and lack clear physical framework for assessing their validity. In this work, we constructed comprehensive datasets from unbiased MD simulations of AuNCs with varying sizes and surface chemistries interacting with multiple blood proteins. These datasets serve as a ground-truth reference for binding-site occupancies for systematic evaluation of predictive models. Comparison of previous interaction energy-based predictions against the ground-truth MD data reveals that many predicted sites exhibit negligible occupancy in these reference simulations. We attribute this discrepancy in part to the choice of training target, as interaction energies do not directly describe binding propensity. To address this limitation, we introduce a more physically grounded learning target based on free energies. We compute free energies of (un)binding for protein-AuNC complexes using adaptive biasing force calculations with the accelerated weight histogram (AWH) method, and use these estimates in binding-site prediction. Unlike interaction energies, free energies are directly related to thermodynamic binding probabilities and are less sensitive to small structural fluctuations. We find that free energy -based targets result in improved agreement with the ground-truth binding site occupancies compared to interaction energy -based approaches, supporting their use in more reliable binding-site prediction models.

A Systematic Comparative Study of TB methods and DFT for Ligand-Protected Nanoclusters

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Ligand-protected metal nanoclusters (MNCs) are nanomaterials with well-defined atomic structures, which can be tuned to produce specific electronic, optical and chemical properties [1]. Typically, the primary computational methods used to study and design novel MNCs are molecular dynamics (MD) simulations and Density Functional Theory (DFT) calculations. However, performing these simulations can be computationally expensive for big and complex systems. Tight-binding (TB) methods offer a computationally efficient alternative while retaining much of the underlying quantum-mechanical description. While DFTB generally provides higher accuracy and predictive power, xTB is broadly applicable without additional parameter development, making it attractive for automated high-throughput workflows. In the present work, we perform a systematic assessment of how these TB methods can be used in ligand-protected nanoclusters studies while defining a workflow that reduces computational cost by orders of magnitude. We investigate electronic properties and geometric features of 64 MNC systems with gold core and a variety of organic molecules in the ligand layer, including thiols, phosphines, alkynes, sulphides and halides. We performed DFT calculations using GPAW software and PBE functional, DFTB2 calculation using DFTB+ software and *auorgap* parameters and xTB, with GFN-1 Hamiltonian using xTB software. Preliminary results show an excellent agreement between DFT and DFTB methods (Fig.1A) with a mean absolute error (MAE) of 0.094 eV, which is within the literature error for HOMO-LUMO (HL) gap calculations [2]. A good agreement is also observed between DFT and xTB methods (Fig.1B), however more outliers were detected (MAE=0.118 eV). For both cases, it was observed that there is a high correlation between the ordering of the gap values (Spearman's ρ and Kendall's τ) which is important for screening applications. For formation energy (FE), a similar pattern was observed, with lower MAE for the DFTB method (Fig.1C and Fig.1D), which both methods were within literature error [3]. For geometry optimisation, xTB method is closer to DFT for the selected structure (Fig.1E). Further analyses are still ongoing, but already, both TB methods have been shown to retain much of the DFT accuracy for the MNC structures studied in this work.

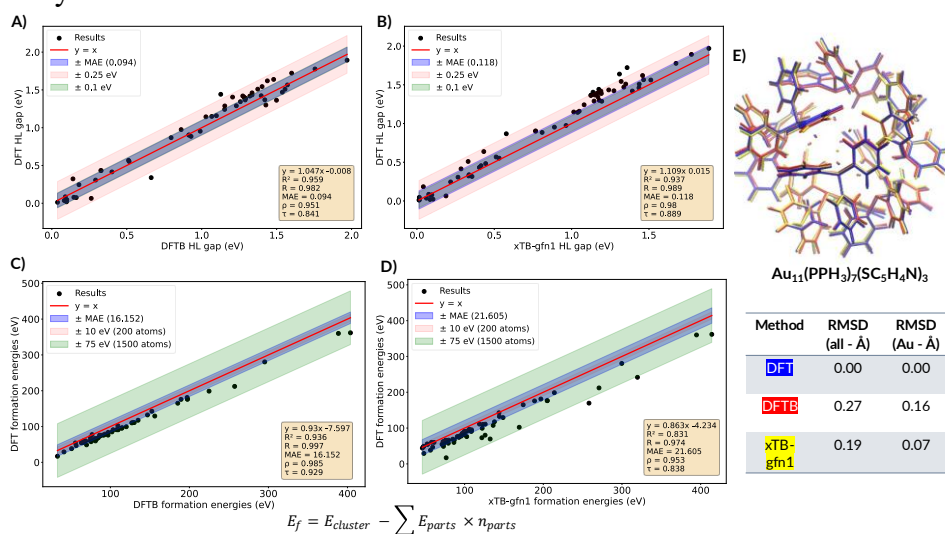


Figure 1: Electronic and geometric comparison. A) HL DFT and HL DFTB. B) HL DFT and HL xTB. C) FE DFT and FE DFTB. D) FE DFT and FE xTB. E) Superimposed geometry optimised structures.

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Photocleavable BODIPY derivatives as peptide-based supramolecular gelators

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Gelation can be controlled with light, in both directions, either in gel formation or gel decomposition. Photoresponsive gelators are molecules that can change their structure or conformation upon light irradiation and thus affect the gelation properties of the resulting residue.[1] One strategy to construct a photoresponsive gelator is to embed a photocleavable group (PPG) in the structure. PPGs are a class of compounds that act as a protecting group, and they can be removed irreversibly by light irradiation [2]. There are only a few examples of low-molecular weight photocleavable gelators containing a PPG, such as coumarin and nitrobenzyl derivatives. [3-4] Gelators with photoresponsivity are potential for applications where controllability of gelation or gel degradation is required, such as in drug delivery.

Here, we aim to synthesize novel peptide-based supramolecular gelators containing a photocleavable BODIPY unit (boron-dipyrromethene, Figure 1) which is sensitive to green light [5]. In gelation studies, we aim to study how gelators will respond to light irradiation either in a gel or in solution, and whether it induces the gelation or gel decomposition (Figure 1). Currently, we are in the synthesis phase, in which the direct coupling of the BODIPY unit to the peptide chain has turned out to be challenging. Hence, we are trying to improve the coupling by varying mono- and dipeptide chains and by embedding different linkers between the BODIPY unit and the peptide chain.

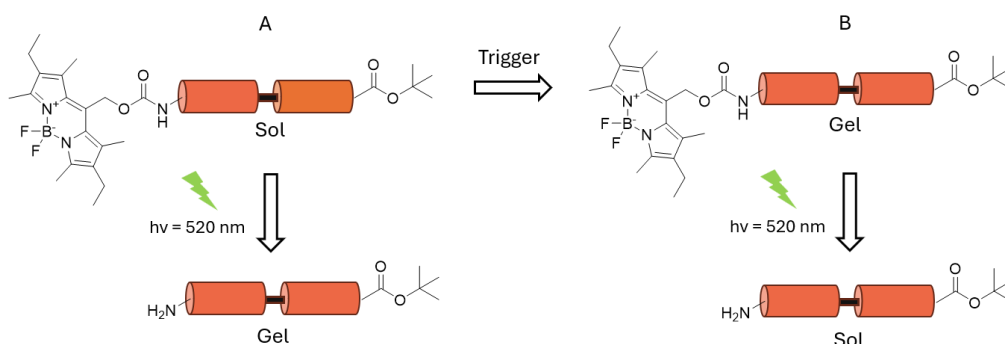


Figure 1. Two possible pathways for photoresponsivity of peptide-based BODIPY gelators. A) Photoinduced gelation or B) photoinduced degradation of the gel due to the removal of the BODIPY unit.

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Understanding hemicellulose-mediated regulation of cellulose microfibril structure using a bacterial model system

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Cellulose microfibrils are the basic building blocks of plant cell walls. They form when individual β -glucan chains come together into semicrystalline microfibrils, which then aggregate further into bundles. This hierarchical supramolecular structure gives the cell wall much of its mechanical strength. Hemicelluloses are thought to play a big part in guiding this self-assembly, shaping the size, shape, crystallinity and packing of microfibrils through non-covalent interactions like hydrogen bonding and non-polar interactions. However, hemicelluloses are polysaccharides that come in many chemical forms, varying in sugar composition, branching, and substitution patterns [1]. In fact, they share a similar β -1,4-linked backbone with an equatorial configuration to cellulose itself, which allows them to align closely with the cellulose fibril surface [2]. However, we still do not have a clear picture of how these differences in branching and substitution actually control fibril assembly at the molecular level. Understanding this link would connect the chemistry of individual polysaccharides to the larger, multi-scale cell wall that plants build. To study this in a more controlled way, we use bacterial cellulose producing *Komagataeibacter xylinus* [3] as a basis for a simplified model system [1,4]. These bacteria produce highly pure cellulose, hence we can introduce well characterized wood hemicelluloses straight into the growth medium and observe how they influence fibril formation, without interference from other cell wall components such as lignin. One of our approaches is capturing this assembly process as it unfolds, from the very first moments of microfibril formation to the emergence of mature bundles. Using transmission electron microscopy and helium ion microscopy, we observe the earliest stages of fibril nucleation in the presence of hemicelluloses, then follow how these fibrils grow, twist, and bundle together as time goes on. This gives us a stage-by-stage view of how hemicelluloses get woven into the growing cellulose structure by offering a rare glimpse into a process analogous to what normally happens out of sight, inside a living plant cell.

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Targeted apoptosis of neurons and brain tumor cells using near-infrared light (BrainRED)

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Targeting specific cell types in the brain is difficult due to the lack of non-invasive methods and technology. This is a problem not only in neuroscience but also in brain cancer treatment, as traditional methods mostly focus on coarsely destroying a region of most interesting/affected cells with lesions, irradiation [1] and/or chemotherapy [2]. Optogenetics aims to control cell function and signaling with light [3]. It has enabled researchers to acquire information, e.g., on neural circuits concerning behavior and learning, although the use of blue light often requires implanting an optical fiber to deep brain tissues [4]. With optogenetic tools that utilize red and near-infrared light (NIR) sensing bacterial phytochromes [5, 6], these implantations are, however, not required. The aim of this research is to generate optogenetic BrainRED tools that induce targeted apoptosis in hippocampal dentate gyrus granule cells (DGC) and in medulloblastoma cells with NIR light. These tools are based on bacterial phytochrome activity that induces the expression of pro-apoptotic proteins. By applying these tools to DGCs in rat models, we expect to reveal how forming new memories in hippocampus occur. These tools will also be used to abolish the medulloblastoma tumor cells without causing any major side effects in overall health and cognition. This is important for adult patients but especially for pediatric patients with developing brains.

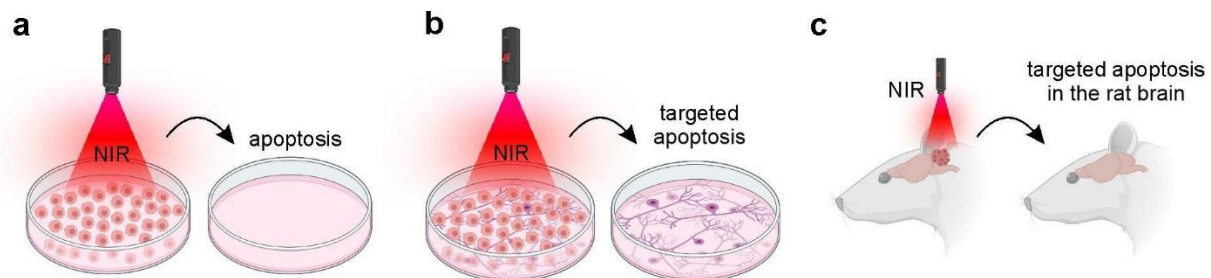


Figure 1: Apoptosis using near infrared light on specific cells. a) Firstly, we induce apoptosis on a specific cell type with NIR light. b) Secondly, we induce apoptosis in specific cells in coculture with BrainRED tool delivered by viral vectors and cell-specific promoters. c) Thirdly, we apply the tools *in vivo* by inducing apoptosis in hippocampal neurons as well as medulloblastoma in rat brain.

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A carbon-nitrogen-oxygen machine-learning potential for direct comparison with 4D-STEM and EELS data on amorphous carbon films

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Machine-learning interatomic potentials have proved remarkably successful for amorphous carbon. Gaussian approximation potentials (GAP) [2,3] for amorphous carbon [4] and its oxygen-rich form [5] reach density functional theory (DFT) accuracy at a cost that allows molecular dynamics on the length and time scales at which amorphous structures form, and reproduce standard characterisation data such as structure factors and photoelectron spectra. Electron microscopy is rarely used this way, yet it resolves what those methods average over: four-dimensional scanning transmission electron microscopy with electron energy-loss spectroscopy gives composition, bonding and bond lengths with depth in sputter-deposited films [1]. Matching simulation to such films, which take up nitrogen as well as oxygen, needs a C, N and O potential yet none exists.

We build a C-N-O GAP from the existing carbon and carbon-oxygen models, augmenting their reference databases in two ways. Dimer and trimer scans supply the N-O two- and three-body reference and the short-range repulsion, which no database contains. C-N-O configurations, absent from every database, are generated by relabelling heteroatoms in equilibrated C-N and C-O geometries and re-computing the energies with DFT. The relabelling targets atoms that already have a like neighbour, producing real N-O contacts rather than N and O sitting apart.

The potential now reaches an overall energy RMSE of 51 meV/atom, reproduces the six pair curves to 0.02–0.19 eV and the diamond and graphite lattice constants to 0.005 Å, and conserves energy to 0.28 meV/atom/ps in dynamics stable to 5000 K. Parameter tuning and model refinement continue, for a more efficient potential: per-class sparse-point quotas, class-dependent regularisation weights, and force-data subsampling that halves the fitting time at no accuracy cost. An active-learning loop across the C-N-O composition simplex is running; its DFT frames will give the first test of generalisation, before simulated and measured reduced density functions are compared.

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Cryogenic Optical Probing of Bound Excitons Toward Spin–Photon Interfaces

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One of the most promising candidates as an integrated and scalable platform for quantum computers is a spin-photon interface in silicon, where there is the possibility of implanting single donors/defects and encoding the information onto their electron or nuclear spins. While novel studies have been conducted around enabling a spin-photon interface using donors in silicon [1], the practical implementation of the optical read-out for single donors that are doped in silicon-on-insulator (SOI) chips remains a challenge. In our work, we demonstrate a customized low temperature optical setup and present our data for measurements on phosphorus-doped bulk silicon in zero magnetic field in both resonant and non-resonant excitation scheme measured in a continuous-flow cryostat. Our experiments provide information and insight on the sensitivity of bound-exciton photoluminescence experiment to the temperature and thermal performance of the sample mounting structure.

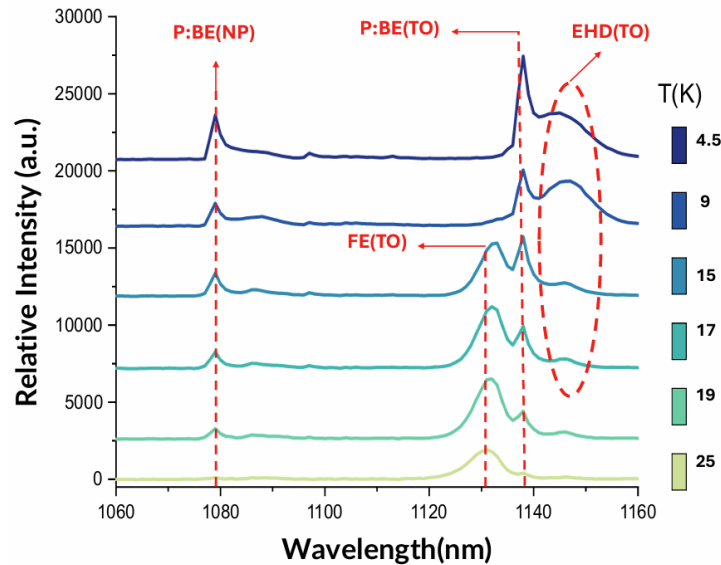


Figure 1. The spectrum of the Phosphorus doped Silicon in temperatures ranging from 4.5-25K, exhibiting the conversion of free-excitonic radiation to bound-exciton radiation by lowering the temperature. The color-bar shows the temperature sensed by a silicon diode close to the sample.

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Investigation of Au₂₂(KCK)₁₆ Nanocluster and Reactive Oxygen Species (ROS) with DFT-MD Simulations

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The interfacial reactivity of atomically precise, biocompatible gold nanoclusters toward molecular oxygen (O₂) is central to understanding their behavior in physiological environments. In this work, we probe the atomistic mechanism of O₂ activation at Au₂₂(KCK)₁₆, a 22-atom gold nanocluster protected by 16 Lysine–Cysteine–Lysine (KCK) tripeptide ligands, combining classical molecular dynamics for configurational sampling with density functional theory-based molecular dynamics (DFT-MD) for electronic-structure evolution [1,3,4]. Rather than a discrete two-electron reduction, O₂ activation at the Au–S(Cys) interface unfolds as a continuous electronic reorganization: triplet O₂ undergoes progressive spin quenching with partial population of its π^* antibonding orbitals, giving rise to a charge-transfer-induced, spin-quenched intermediate with a near-zero magnetic moment and moderate O–O elongation, before evolving into a fully spin-paired, peroxide-like state with substantial O–O bond extension [2].

Time-resolved magnetic moments, O–O bond lengths, frontier orbital energies, and Bader charge distributions consistently trace this pathway. Projected density-of-states analysis identifies interfacial Au(d)–O₂(π^*) hybridization as the electronic driving force, while charge partitioning attributes the transferred electron density predominantly to the gold core [5,6]. These results show that thermal fluctuations alone are sufficient to drive charge transfer to O₂ at the nanocluster surface, pointing to a plausible route for reactive oxygen species generation in oxygen-rich biological environments.

Keywords: Gold nanoclusters, Reactive oxygen species, DFT-MD, Charge transfer

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From Crystal Structures to K_1 – A First-principles Database of Magnetocrystalline Anisotropy Constants

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Magnetocrystalline Anisotropy (MCA) [1], quantified by the anisotropy constant (K_1), governs the performance of permanent magnets. Materials with higher MCA are more resistant to demagnetization by stray fields and thermal fluctuations, making them 'harder' magnets with higher coercivity and better suited for various high performance applications. Rare-earth metals achieve high K_1 through strong spin-orbit coupling (SOC), while rare-earth free compounds have intrinsically lower SOC and tend to show lower anisotropy. This makes K_1 an important figure of merit in evaluating rare-earth free permanent magnets, but the high computational cost of calculating it from first-principles limits the pace at which large chemical spaces can be screened.

Although ML surrogate models could in principle accelerate this screening, no models reported in the literature to date do it reliably across diverse chemistries. Existing models are usually limited to narrow chemical spaces and fixed structural prototypes, both because of a lack of large-scale databases and because MCA is highly sensitive to electronic structure and SOC effects, making it challenging to model.

To address these gaps, we construct a database of nearly 4200 crystal structures and their corresponding K_1 values, spanning a wide range of chemical systems, using high-throughput DFT workflows. To our knowledge, this is the first such database combining chemical diversity with explicit structural information on a large scale, intended to be made publicly available, in a form suitable to approach the problem using machine learning. This dataset is then utilised to train machine-learning models on three complementary K_1 prediction tasks given only a crystal structure – (a) K_1 regression, (b) predicting the sign of K_1 , and (c) predicting $K_1 > 1 \text{ MJ/m}^3$. Among these, the classifier predicting the sign of K_1 has proven effective, with precision exceeding 90%, making it a valuable tool for high-throughput workflows by allowing efficient screening of materials before committing to expensive DFT calculations.

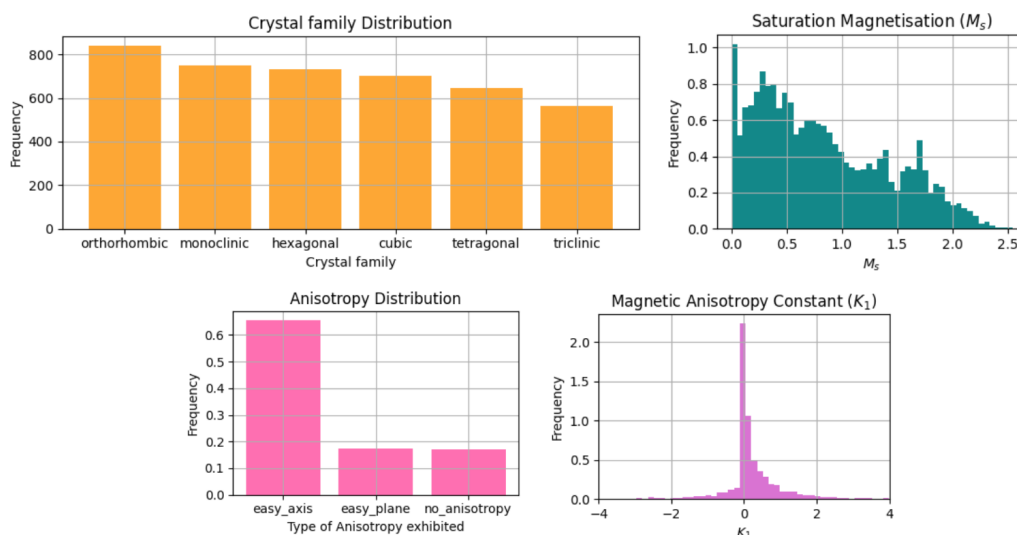


Figure 1: Statistical distributions of various quantities evaluated over the entire dataset.

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Dynamic Protonation as a Missing Piece in Protein–Protein Binding Free Energy Calculations

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Despite rapid progress in molecular modeling, driven by advances in machine learning and computational power, achieving a predictive theoretical description of protein–protein interactions remain a major challenge. A critical yet often overlooked factor is the dynamic nature of residue protonation, which fundamentally influences intermolecular interaction mechanisms.

To overcome this limitation, we incorporate a recently introduced dynamic protonation approach into molecular simulations of protein complex dissociation by combining constant-pH molecular dynamics (CpHMD) [1-3] with the adaptive-biasing accelerated weight histogram (AWH) method [4-5]. This integrated approach enables the investigation of how protonation dynamics modulate binding free energy landscapes.

We demonstrate that coupling CpHMD with AWH significantly accelerates the convergence of the potential of mean force (PMF) compared to conventional simulations. Moreover, the inclusion of protonation dynamics leads to a smoother free energy profile and facilitates escape from local minima, improving sampling efficiency and robustness of the calculated binding free energies. All simulations were performed in GROMACS within a unified molecular dynamics workflow.

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Playing ‘Hide & Seek’ at Atomic-scale

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The layered transition-metal telluride compound TaCo₂Te₂ has attracted growing attention because of its fermionic band degeneracy, air-stability, and low-dimensional crystal structure [1,2]. In this work, we investigate the structural, electronic, and magnetic properties of TaCo₂Te₂ using a combination of experimental characterization techniques and density-functional theory calculations. TaCo₂Te₂ possesses a distorted crystal structure in which the top Te atoms occupy three nonequivalent positions, leading to distinct structural appearances depending on the scanning probe technique employed. In particular, constant-current scanning tunneling microscopy (STM) images reveal a square-like surface structure, whereas constant frequency-shift atomic force microscopy (AFM) images display a pseudo-hexagonal arrangement. Furthermore, the electronic properties of TaCo₂Te₂ is examined using scanning tunneling spectroscopy (STS), and the obtained results are consistent with complementary angle-resolved photoemission spectroscopy (ARPES) measurements.

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Geometry-Driven Enhancement of Light-Matter Coupling in Molecular Microcavities

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Strong light-matter coupling in optical microcavities produces hybrid light-matter states, known as polaritons, with potential applications in molecular photonics, energy transfer, and photochemistry [1]. The collective coupling strength, g , is related to the number of molecules, N , interacting with the confined optical mode with an effective mode volume of V , through $g \propto (N/V)^{1/2}$, suggesting that stronger optical confinement, i.e. smaller V , should enhance the interaction. However, our experimental observations and complementary simulations show that thinning of the metallic mirror of a Fabry-Pérot cavity, i.e. increasing the mirror transmittance, can increase the observed polariton splitting, despite the fact that the increased leakage reduces the optical confinement and increase V . This counterintuitive behavior indicates that the system response cannot be understood through geometric confinement alone.

Cavity and molecular dissipation originate from physically distinct mechanisms, although their respective linewidths enter together into conventional strong-coupling criteria [2,3]. Molecular linewidth and oscillator strength can also determine whether individual transitions reach the strong-coupling regime [4]. Here, we independently vary cavity linewidth, molecular linewidth, oscillator strength, and top-mirror thickness and examine their effects on polariton splitting and molecular-layer absorption. We find that cavity and molecular broadening modify the polaritonic response differently, while mirror thickness further influences cavity leakage, interference, field distribution, and the effective light-matter interaction. These results show that changes in observed polariton splitting cannot be interpreted solely through a single effective loss or coupling parameter and highlight that the physical origin of dissipation, not just its magnitude, is a key consideration in the design of molecular microcavities.

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DNA-Based Logic Gated Circuits for Sensing and Memory in Circulation Mimicking Systems

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A double strand DNA-based system enables stimulus-triggerable memory via biomolecular interactions. The sensing element comprises structure-responsive DNA aptamers that bind specific biomolecules, like ATP [1], causing analyte-induced structural changes that displace a unique strand [2]. This strand enters a DNA logic gated circuit that remembers previously encountered analytes, executing simple Boolean algebra and providing DNA strands as output [3]. The displaced strand then inputs to the reporter, displacing a double strand reporter and generating fluorescent output. This fluorescence monitors the strand displacements and overall network performance. The system is incorporated into a microfluidic channel, simulating small-scale fluid circulation and biosystem functionality [4]. These results open new model systems to simplify and study ways to mimic closed circulatory systems in biological organism.

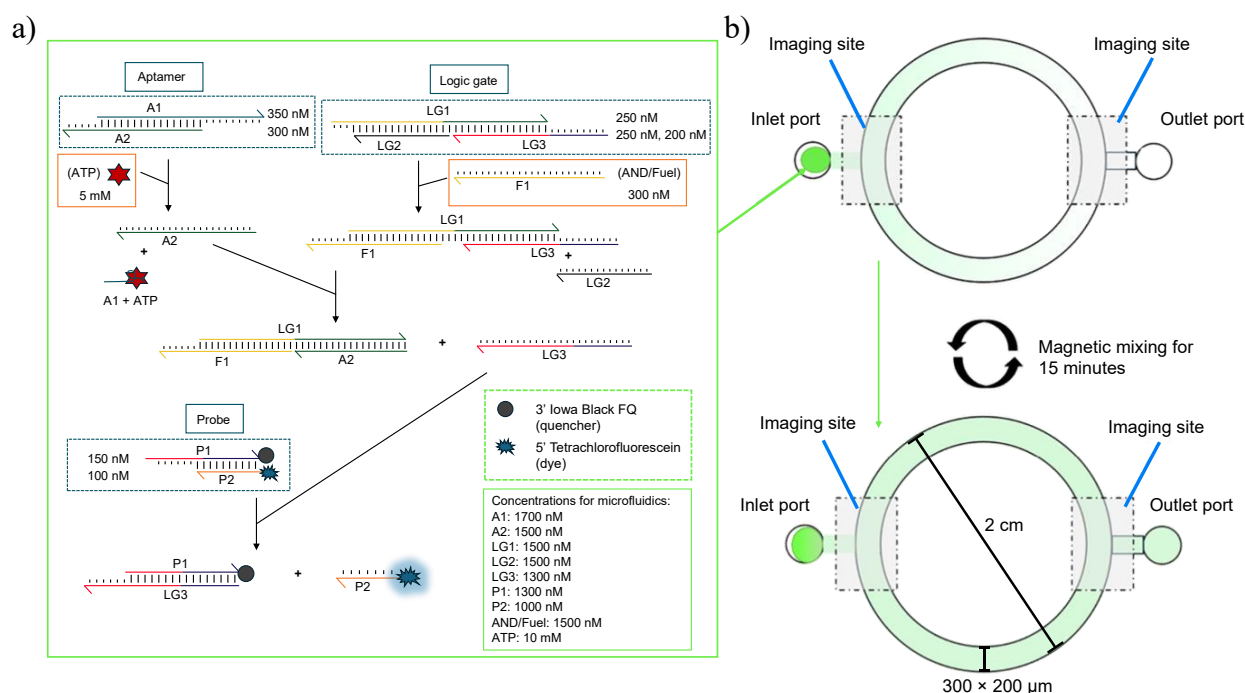


Figure 1. (a) Schematic illustration and DNA strand concentrations for the strand displacement reactions. Symbols for the dye and quencher molecules and DNA strand concentrations for a microfluidic experiment are also listed. (b) Schematic illustration of a microfluidic channel with imaging sites and dimensions shown. The stirring mixes the DNA strands and analytes evenly inside the channel, as seen with spreading green color.

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The Interplay Between Aging, Physical Activity and Immune Cells in Lynch Syndrome Cancer Risk Regulation

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Lynch Syndrome (LS) is one of the most common hereditary cancer predispositions caused by mutations in DNA mismatch repair genes. Despite the lifelong increased cancer risk, not all LS carriers develop cancer. Immune cell function plays crucial role in cancer prevention as well as in regulation of cancer progression, while ageing causes deceleration of immune responses and drives immune cell composition towards low-grade inflammation. However, genetic factors, such as LS, and environmental factors can cause variance in this age-related reshaping of immune system. Lifestyle factors, such as physical activity (PA), may improve immune system balance: Exercise induces rapid mobilization of immune cells and regular PA enhances immune cell function and anti-inflammatory properties of immune cells. Nevertheless, the underlying associations between aging, PA and immune cells in LS cancer risk regulation are not comprehensively studied.

In this study, we aim to uncover these associations by investigating circulating immune cell profiles in cancer free LS carriers and non-carriers aged between 25-78 years old with different habitual PA backgrounds. We use antibody panel designed for flow cytometry of immune cells to study the differences in the number and distribution of 13 different immune cell subtypes. Our hypothesis is that in LS the immune cells involved in early anticancer surveillance are elevated, and that immune ageing is accelerated in LS carriers. However, we expect higher habitual PA to mitigate this process. This study will provide elucidative information of how PA affects immune resilience in LS during aging.

pH controlled self-assembly of DNA origami lattices on silicon wafer for bottom-up nanofabrication

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Plasmonic nanostructures have attracted increasing attention in photonics due to their potential as components of novel quantum optics [1] and metamaterials including negative refractive index (NIM) [2,3] by using so-called fishnet structures [4]. DNA has emerged as a promising material for fabricating such nanostructures due to its robust self-assembly and functional properties [5]. For example, cross-shaped DNA origami can be used as a building block to fabricate fishnet-type lattices on substrates such as mica [6].

Since further processing on mica is not possible with common processes, alternative surfaces like silicon have been investigated. Earlier, we have developed a fabrication methodology to self-assemble a closely spaced polycrystalline two-dimensional fishnet lattice on a silicon substrate with an average domain size of about a micrometer [7]. Recently, we have optimized to double the average domain size by changing different ionic environments, temperatures and origami-origami bonding strengths and achieved the average domain size of $\sim 2\ \mu\text{m}$ and even single-crystal lattices up to diameter of $5\ \mu\text{m}$ [8].

All the above optimization was done in pH 8. Therefore, the project was extended to investigate how pH effects lattice assembly and DNA origami stability across pH 3-11. The DNA origami denatured at pH 11 but in contrast survived even at pH 3. The most stable lattices were found at slightly basic pH 8-9. The results indicate that lattice formation is sensitive for pH. Outcome of this research will establish a optimum pH range for all the future studies of this system.

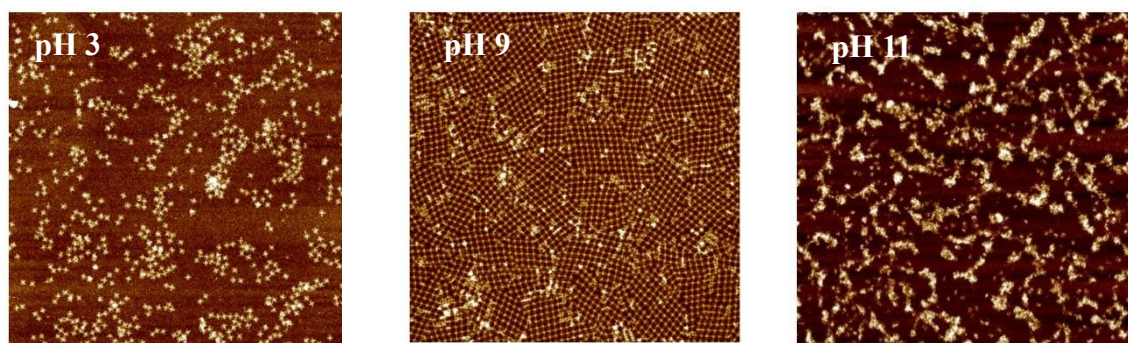


Fig. 1: Atomic force microscope (AFM) images of DNA origami fishnet-type lattice on silicon with different pH values.

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Toward reliable spectroscopic analysis of vibrational strong coupling in polaritonic chemistry

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Strong coupling between molecular vibrations and confined electromagnetic modes of infrared cavities gives rise to hybrid light–matter states known as vibrational polaritons, which have been reported to modify ground-state chemical reactivity [1,2]. However, the physical origin of these effects remains highly debated, especially considering recent difficulties in reproducing several landmark experiments [3,4]. Reported alterations of chemistry under vibrational strong coupling, such as reaction rates, product distributions, intermolecular forces, and cavity-mediated vibrational energy transfer, raise skepticism due to multiple irreproducible attempts [5,6]. Therefore, robust and standardized protocols for reproducible vibrational strong coupling experiments are essential in polaritonic chemistry.

In this context, we have investigated vibrational polaritons through a combined experimental and theoretical approach. We identify several overlooked experimental pitfalls, like transient changes in cavity thickness upon reactant introduction, which can strongly distort apparent reaction kinetics and mimic signatures often attributed to vibrational strong coupling [7]. In addition, we also identify the technical drawbacks of a microfluidic optical microcavity system, especially in the case of extracting chemical reaction rates, and try to optimize it through UV–Vis measurements, by eliminating artifacts that distort observed absorption peak positions and amplitudes. By identifying these pitfalls, our work lays the foundation for more robust analyses and reliable measurements in polaritonic chemistry. Our findings aid in establishing best practices for carrying out robust future investigations of cavity-modified chemistry.

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Antiviral boreal tree bark compounds and antiviral surfaces

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There is an urgent need to develop more novel methods to combat enteroviruses. Broad-spectrum antivirals, capable of inhibiting multiple virus strains or even species, have gained much attention, as they not only offer direct medical treatment but can also be deployed in more novel methods, such as antiviral surface materials, disinfectants, and material coatings used to lower viral transmission in the environment. These are desperately needed against enteroviruses as they are exceptionally persistent in the environment and highly resistant to many conventional disinfectants.

Tree bark is rich in bioactive compounds, including terpenes and polyphenols, and serves as a sustainable, low-cost, and abundantly available forest industry side-stream. Prior studies in our group have explored how solid wood surfaces and more purified compounds extracted from spruce bark are able to inhibit both enteroviruses and coronaviruses.

My research seeks to characterize and identify antivirally active compounds from the bark of multiple boreal tree species, together with studying their mechanisms of action. The end goal is to develop and test antiviral surface materials. My first study showed that crude bark extracts from seven different tree species displayed good or modest antiviral activity against CVA9, EV-A71, and HCoV-OC43. In this study, we also identified their differing molecular profiles with many promising compounds from the bark extracts. Interestingly, we could not use total phenolic content to predict antiviral activity. We have begun further fractionation of the crude extracts, and indeed most of our current fractions have demonstrated good antiviral activity, suggesting the presence of multiple antivirally active compounds that we are trying to characterize and further isolate.

Antiviral Activity and Metabolite Profiling of Finnish Berries

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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, despite the numerous findings reported to date, a broad and systematic screening of berries against multiple viruses has not yet been comprehensively performed. Therefore, the present study was undertaken to identify new antiviral activities and to gain further insight into the metabolic profiles potentially contributing to these activities.

22 berry samples collected from Finland were tested against enteroviruses CVA9 and CVB1, and seasonal human coronavirus OC43 using cytopathic effect assay. Principal component analysis revealed correlations between total polyphenol phenolic content or total anthocyanin content, and the antiviral activities (Figure 1). Feature-based molecular networking analysis enabled annotation of 30 different metabolites, including anthocyanins, flavonoids, triterpenes, phenolic acids and diverse glycosidic compounds.

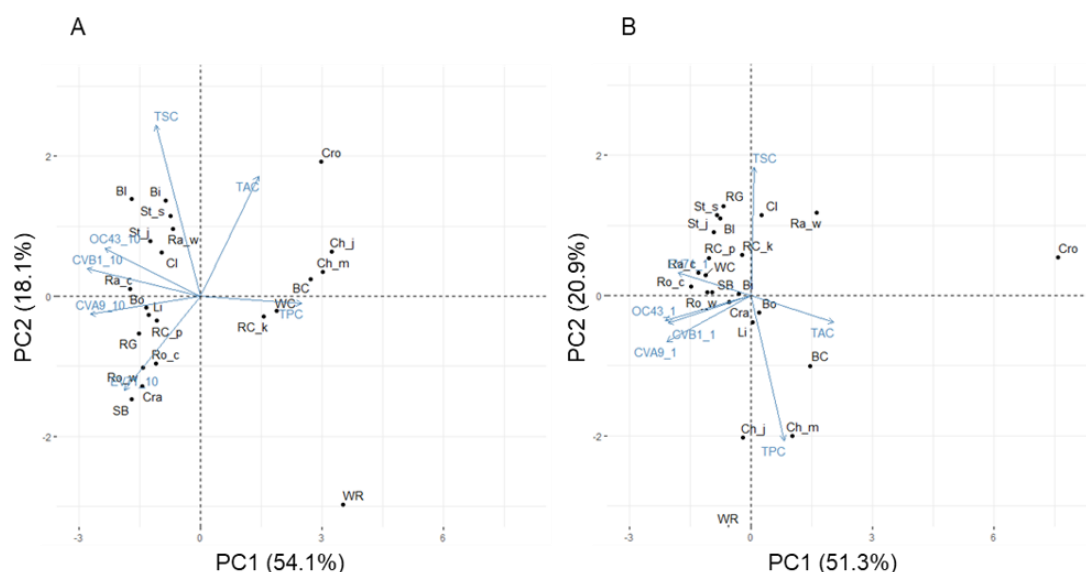


Figure 1: Principal component analysis (PCA) biplot showing total phenolic content (TPC), total anthocyanin content (TAC), total sugar content (TSC), and antiviral activities against enterovirus 71 (EV71), human coronavirus OC43 (OC43), coxsackievirus A9 (CVA9), and coxsackievirus B1 (CVB1) in berry extracts at 10 mg/g DW (A) and 1 mg/g DW (B).

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Towards metasurfaces by DNA-assisted lithography

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In the past decade, DNA origami has become one of the most used building blocks in self-assembled materials at the nanoscale [1]. Using DNA origami as tiles, large 2D lattices have been assembled with different techniques [2]. In our recent work, we have demonstrated that within certain ionic conditions the blunt-ended Seeman Tile [3] origami forms ordered 2D lattices on top of silicon [4] as shown in Figure 1b. These lattices can be further utilized in lithography processes, i.e., DNA assisted lithography (DALI) [5] (shown in Figure 1). Our main goal is to fabricate a multilayered metamaterial surface with a negative refractive index within the visible range [6] to enable novel applications such as perfect lensing, optical filters, optical cloaking and more in a cost-effective manner.

For the fishnet DNA origami lattices, we have already demonstrated the DALI process till midway, i.e., growing silicon dioxide using the DNA lattice as a mask for the following etching step. Although further improvement of the uniformity and thickness of the oxide is still needed. Unlike in the original DALI, we now require a high precision etch process with high Si/SiO₂ selectivity and anisotropic etch profile (no undercut) to avoid the collapse of the mask. Etching has already been tested in cryogenic temperatures with SF₆ based processes but higher etching contrast between Si and SiO₂ while keeping the profile is still needed. Currently, we are optimizing an HBr etching process in higher temperatures. Finally, we will use the etched pattern as an evaporation mask for the metallic-dielectric multilayered nanostructures.

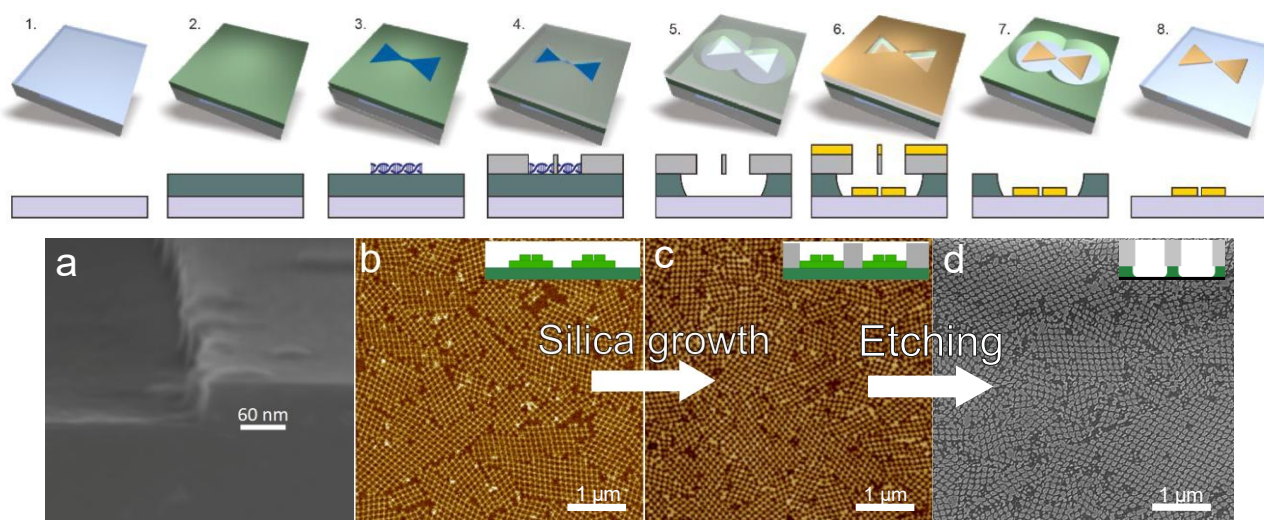


Figure 1: DNA assisted lithography steps [5]: 1. Substrate, 2. Si growth by Chemical Vapor Deposition (CVD), 3. Origami deposition, 4. SiO₂ growth by special CVD, 5. Isotropic Si etching by Reactive Ion Etching (RIE), 6. Au deposition by evaporation, 7. Lift-off by HF-HCl wet etching, 8. Removing of Silicon by RIE. a) SEM image of e-beam lithography sample showing the etch profile. b) AFM image of Seeman Tile fishnet-type lattice deposited on a silicon substrate. c) Similar DNA lattice after SiO₂ growth. d) SEM image of an etched DNA lattice.

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Synthesis of 5-hydroxymethylfurfural using sulfonated calix[4]arene in brine and rapid reaction monitoring with MEKC

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5-Hydroxymethylfurfural (HMF) is a platform chemical created primarily from dehydration of C6-carbohydrates (Figure 1a).¹ HMF has multiple important derivatives, such as 2,5-furandicarboxylic acid that has been posed to replace terephthalic acid in the production of polyesters², and 2,5-dimethylfuran that has potential as a biofuel³. Various acids, solvents and feedstocks have been utilized in the synthesis of HMF.¹ Sulfonated calixarene (sC4A) is a macrocyclic organocatalyst that has been used in various syntheses⁴, including the dehydration of fructose into HMF⁵.

HMF readily decomposes into levulinic acid (LA) and insoluble humin material. Even though LA is a platform chemical⁶, its creation is problematic due to the loss of the furan-ring functionalization. Humins can clog machinery in industrial processes and prevent conversion by trapping feedstock into its matrix.⁷ Thus it is important to limit side product generation in HMF synthesis.

D-(–)-fructose was dehydrated in brine in the presence of various organic and mineral acids. HMF and LA were isolated from reaction mixture with liquid-liquid extraction using ethyl acetate and yields were determined with ¹H qNMR. The production of HMF over time was quantified with micellar electrokinetic chromatography (MEKC). The decomposition of HMF to LA in presence of acid was investigated. The host-guest interactions between sC4A and HMF were explored at different temperatures.

The highest isolated HMF yield of 32.7 ± 5.4% was achieved from dehydration of fructose with sC4A (Figure 1b). MEKC was successful in quantifying HMF at the 0.01–10 mM range with LOD and LOQ of 0.003 mM and 0.009 mM, respectively. Decomposition of HMF in the presence of sC4A created the least amount of LA, compared to other acids screened. sC4A binds HMF in D₂O.⁸

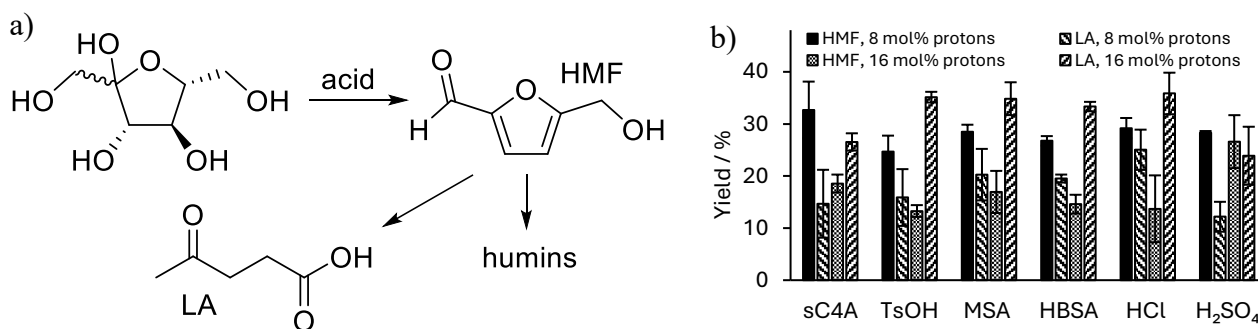


Figure 1a) Synthesis of HMF from fructose and its decomposition into LA and humins and b) yields of HMF and LA from dehydration of fructose with various acids in brine.

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Heterogeneity and spatial distribution of cancer-associated fibroblasts in colorectal cancer

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Colorectal cancer (CRC) is one of the most common cancers worldwide [1]. Within the CRC tumour microenvironment, cancer-associated fibroblasts (CAFs) represent one of the most prevalent cell populations [2, 3]. The considerable phenotypic diversity and functional plasticity of CAFs have made it challenging to fully define the contribution of CAFs in tumour progression and clinical outcomes [4, 5, 6].

We utilised a custom 8-plex immunohistochemistry assay combined with machine learning-based image analysis to quantify SMA-, FAP-, MCAM- and PDPN-positive CAFs and CD45-positive immune cells in 935 CRCs. We evaluated their densities, spatial distribution, clinicopathological associations, and prognostic significance.

High overall CAF density associated with poorer cancer-specific survival (HR for Q4 vs. Q1 1.84, 95% CI: 1.28–2.64), whereas high immune cell density correlated with improved outcomes (HR for Q4 vs. Q1 0.24, 95% CI: 0.16–0.36). Variation in both CAF and immune cell densities were observed according to tumour anatomical location and MMR status. Furthermore, prognostic associations varied between distinct CAF phenotypes, and particularly MCAM- and PDPN-expressing CAFs were linked to improved survival.

These findings suggest that CAFs in CRC exhibit substantial prognostic heterogeneity, highlighting the limitations of using total CAF abundance as a single measure of clinical relevance. The findings underscore the value of comprehensive spatial profiling of CAF subpopulations together with immune cells when assessing their contribution to disease progression.

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Avoided crossings in spin-boson systems: consequences for adiabatic state preparation

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Avoided crossings in the correlated many-body spectrum play a central role in determining the conditions for adiabatic state preparation in interacting quantum systems. We investigate this connection in finite spin-boson systems by combining exact diagonalization of the many-body spectrum with time-dependent simulations of adiabatic switching protocols. By comparing the adiabatically prepared state with the exact ground state, we determine the switching times required for reliable preparation as a function of the spin-boson coupling strength and bosonic mode structure. We show that regions of small many-body level-spacings, associated with avoided crossings, impose the strongest constraints on adiabatic preparation and explain the observed dependence of the required switching times on the interaction strength. Furthermore, while the ground-state energy follows the overall spectral trends, local observables such as the Pauli matrix expectation values exhibit additional non-monotonic behavior arising from the coherent oscillations in finite systems.

Ultrafast photoactivation dynamics of phytochrome proteins under blue-light excitation

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Phytochromes are photoreceptor proteins that allow their host organisms to respond to the light environment. They covalently bind bilins that function as their chromophores and initiate the photoreaction leading to structural changes in the protein and ultimately changes in biological activity. Inherently, phytochromes interconvert between two spectrally distinct states known as Pr and Pfr. While they are commonly known as red-light photoreceptors, they also absorb in the blue region in the Soret-band. The Soret-band-initiated excitation dynamics of phytochromes are less studied but can reveal new possibilities to drive their photoactive reactions.

We applied ultrafast absorption spectroscopy to understand the photoactivation of phytochromes on the timescale where the first intermediates are formed. We investigated whether variations in the binding pocket influence excited-state relaxation and chromophore isomerization by comparing three truncation constructs of phytochrome from *Deinococcus radiodurans* (DrBphP) using femtosecond transient absorption spectroscopy with Soret-band excitation. The resulting spectra show that the excited state kinetics remain very similar to those of the Q-band excitation and are consistent across the applied fluence range, indicating a broader usable dynamic range for excitation powers. These findings provide an alternative experimental approach for studying excitation power dependence and excitation dynamics in canonical photoconversion pathways of phytochrome proteins, to be used for example in time-resolved X-ray crystallography experiment.

Disentangling Optical Filtering from Modified Molecular Dynamics under Strong Coupling

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Changes in steady-state fluorescence and photochemical reactivity under strong light–matter coupling are frequently attributed to modified molecular dynamics [1–3]. However, cavity-modified absorption can produce similar signatures [4], making a quantitative passive-optics benchmark essential. Here, we refine our earlier passive-filtering model [5] using a new five-concentration series of metal-clad microcavities containing 10-hydroxybenzo[*h*]quinoline (HBQ) in a slightly different cavity geometry. The earlier model combined the bare-molecule excitation spectrum with total cavity absorption to predict fluorescence excitation spectra under strong coupling [5]. Here, we refine the absorption contribution by fitting a transfer-matrix model (TMM) to experimental cavity absorption and extracting the absorption specifically in the HBQ-containing layer. This layer-resolved absorption alone reproduces nearly all of the dispersive structure in angle- and wavelength-resolved fluorescence excitation maps:

$$\text{Exc}_{\text{pred}}^{(0)}(\lambda, \theta) \propto A_{\text{HBQ, cav}}^{\text{TMM, L2}}(\lambda, \theta).$$

Across the five cavities, this prediction gives a median normalized-map root-mean-square error (RMSE) of 0.071. Full-stack absorption performs worse because metal losses compromise its sensitivity to molecular absorption.

Although normalized absorption and fluorescence excitation coincide in dilute HBQ solution [5], concentrated HBQ/PMMA films show wavelength-dependent fluorescence per absorbed photon. We account for this using the corresponding uncoupled-film ratio:

$$\text{Exc}_{\text{pred}}(\lambda, \theta) \propto \underbrace{\frac{\text{Exc}_{\text{film}}(\lambda)}{A_{\text{film}}(\lambda)}}_{\eta_{\text{film}}(\lambda)} A_{\text{HBQ, cav}}^{\text{TMM, L2}}(\lambda, \theta).$$

With this correction and spectral broadening, taking into account the roughness induced inhomogeneous broadening in the cavity, the median normalized-map RMSE improves to 0.051 over the valid spectral region. Because η_{film} has no cavity-angle dependence, it refines only the spectral envelope, while molecular-layer absorption determines the dispersive structure. No polariton-branch-specific term is required to reproduce the measured excitation maps. The refined analysis retains our earlier physical interpretation while replacing total cavity absorption with layer-resolved molecular absorption. Strong-coupling effects on chemistry inferred from total cavity absorption should therefore be reassessed using layer-resolved absorption. Our results establish molecular-layer absorption as the primary optical benchmark for cavity fluorescence excitation: dispersive structure in steady-state excitation spectra alone is insufficient evidence for modified molecular dynamics.

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Unravelling the role of DNA positioning and interactions in herpesvirus reactivation

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Herpes simplex-virus type 1 (HSV-1) is a significant global health issue affecting ~70% of the world's population and there is no cure or vaccine against the virus. The primary lytic infection of HSV-1 occurs in epithelial cells, after which the virus remains in the nuclei of peripheral neurons in a life-long latency with occasional reactivation periods and asymptomatic intervals. During reactivation, the latently infected cell re-enters the lytic cycle and starts to produce infectious viruses, leading to infection at the primary infection site. Lytic HSV-1 infection modulates the structure of the host cell nucleus, for example altering the chromatin organization and forming phase separated condensates called viral replication compartments, but the mechanisms regulating the reactivation of the virus are not fully understood.

To study the mechanisms regulating viral reactivation, we utilize LUHMES (Lund human mesencephalic) cells, which are human neuronal cells that can be differentiated to post-mitotic neurons. These cells are a valuable cell model for HSV-1 studies as they can be latently infected with HSV-1, and reactivation can be efficiently induced [1]. Furthermore, the virus can be studied in human cells that resemble the neuronal cells where the virus remains latent in the human host.

This project aims to understand the intranuclear mechanisms of herpesvirus reactivation and how it effects the organisation and dynamics of host chromatin. The research will be conducted using an interdisciplinary approach that combines cell biology and biophysics with advanced imaging techniques, protein structure prediction algorithms, and biophysical modelling.

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Modeling Strong Light–Matter Coupling in Plasmonic Nanocavities

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Over the past decade, strong light–matter coupling has emerged as a powerful strategy for controlling photophysical and photochemical processes[1]. Through the formation of polaritonic states from the hybridisation of molecular excitations with confined electromagnetic modes in cavities, this regime enables the reshaping of potential energy surfaces, facilitates energy transfer, and enhances light harvesting in optoelectronic platforms, motivating extensive experimental and theoretical research[2–3].

However, experimental progress has been hindered by the lack of a predictive theoretical framework capable of quantitatively describing strong coupling in non–ideal systems. In Fabry–Pérot cavities, as the number of molecules increases, numerous dark states (that do not couple directly to the cavity mode) emerge and complicate the excited state dynamics[4].

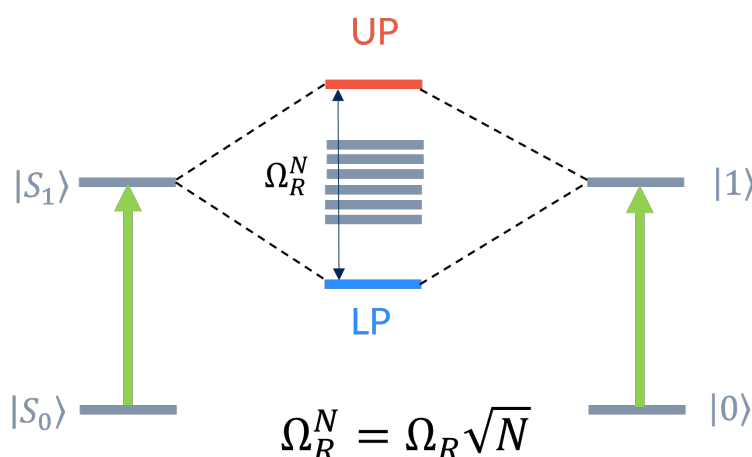


Figure 1: Schematic representation of molecule excitation and cavity mode hybridisation originating polaritonic states (upper UP and lower LP polariton). The energy difference between LP and UP is also known as Rabi splitting Ω_R^N and is proportional to the N number of molecules in the cavity. Dark states are appreciated in the middle of polaritons.

To reduce collective effects and access the strong coupling regime with fewer molecules, alternative architectures such as surface plasmon nanocavities have been proposed[5]. Their extreme electromagnetic field confined in small volumes opens the possibility of single– or few–molecule strong coupling, but requires theoretical descriptions beyond standard cavity quantum electrodynamics.

The development of all–atom approaches that enable more realistic computational simulations closer to experimental results requires a description of the photonic properties of coupled molecular systems, both within and outside the cavity. My talk focuses on advances in the study of these properties, with the aim of applying them to research in the strong coupling regime.

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Does strong light matter coupling really enhance the ultrafast charge transfer?

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Charge transfer (CT) processes in donor–acceptor systems play a central role in photochemical and optoelectronic applications. However, the microscopic factors governing ultrafast CT and their modification in optical cavities remain incompletely understood. Recent experiments on the PM605–TCNQ donor–acceptor system have reported ultrafast CT on a timescale of approximately 150 fs in the absence of a cavity. Upon coupling the molecular system to an optical cavity, the energetic driving force for CT is reduced to approximately 0.5 eV, while the CT process is further accelerated. The origin of this enhancement remains unclear: it may arise from genuine modifications of molecular properties induced by strong light–matter coupling, such as changes in free-energy landscapes, electronic couplings, and nonadiabatic pathways, or may instead be associated with modified optical excitation and absorption conditions in the cavity.

In this work, we investigate the microscopic factors underlying ultrafast CT in the PM605–TCNQ system outside the cavity by combining excited-state electronic-structure calculations with nonadiabatic surface-hopping simulations. We then employ the transfer-matrix method (TMM) to model the distributed Bragg reflector (DBR)-based cavity and determine the photonic modes available for coupling with the molecular transitions. The resulting light–matter interaction is described using a model to investigate the strongly coupled molecular–photonic system and its influence on CT dynamics. Finally, the microscopic simulation results will be interpreted within simplified theoretical frameworks, including Marcus theory and Fermi's golden rule, to establish connections between molecular properties, light–matter coupling, and the observed macroscopic CT rates.

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Investigation of Au₂₂(KCK)₁₆ Nanocluster and Reactive Oxygen Species (ROS) with DFT-MD simulations

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The interfacial reactivity of atomically precise, biocompatible gold nanoclusters toward molecular oxygen (O₂) is central to understanding their behavior in physiological environments. In this work, we probe the atomistic mechanism of O₂ activation at Au₂₂(KCK)₁₆, a 22-atom gold nanocluster protected by 16 Lysine–Cysteine–Lysine (KCK) tripeptide ligands, combining classical molecular dynamics for configurational sampling with density functional theory-based molecular dynamics (DFT-MD) for electronic-structure evolution. Rather than a discrete two-electron reduction, O₂ activation at the Au–S(Cys) interface unfolds as a continuous electronic reorganization: triplet O₂ undergoes progressive spin quenching with partial population of its π^* antibonding orbitals, giving rise to a charge-transfer-induced, spin-quenched intermediate with a near-zero magnetic moment and moderate O–O elongation, before evolving into a fully spin-paired, peroxide-like state with substantial O–O bond extension. Time-resolved magnetic moments, O–O bond lengths, frontier orbital energies, and Bader charge distributions consistently trace this pathway. Projected density-of-states analysis identifies interfacial Au(d)–O₂(π^*) hybridization as the electronic driving force, while charge partitioning attributes the transferred electron density predominantly to the gold core. These results show that thermal fluctuations alone are sufficient to drive charge transfer to O₂ at the nanocluster surface, pointing to a plausible route for reactive oxygen species generation in oxygen-rich biological environments.

Efficient scanning-probe spectroscopy using Wannier-based non-equilibrium Green's functions

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Scanning tunneling microscopy and spectroscopy (STM/STS) provide powerful tools for probing electronic properties at the atomic scale. On the theoretical side, density functional theory (DFT) and Wannier-based methods enable realistic first-principles descriptions of complex nanosystems. However, modeling nonequilibrium transport remains challenging, particularly in superconducting hybrid systems where particle-hole correlations must be treated explicitly. Here, we present a workflow combining Wannierized first-principles electronic structure calculations with the nonequilibrium Green's function formalism for efficient simulations of STM experiments [1]. The approach builds on standard DFT packages to construct compact transport Hamiltonians that retain the electronic properties of realistic materials. Superconductivity is incorporated through an effective pairing potential within the Nambu-spinor formalism, while the coupling to the STM tip and substrate electrodes is treated within the wide-band limit approximation. Within this framework, transport quantities such as current-voltage characteristics can be evaluated in closed analytical form. The method provides a unified and computationally efficient approach for modeling superconducting hybrid nanostructures with spin-orbit coupling, magnetic textures, and spin polarization.

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Ultrasensitive ratiometric fluorescent detection of enteroviral RNA via enhanced electron transfer between carbon dots and intercalating fluorophores

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Facilitating real-time, in situ detection of viral RNA activation enables advancements in antiviral research and understanding the mechanisms of viral entry for healthcare applications. Fluorescence nanoparticles, particularly carbon dots (CDs), a quasi-spherical fluorescent carbon-based nanomaterial, have proven to be promising tools for precise optical sensing of bioanalytes like viruses, allowing further research and development for various biological applications.

In our previous work, we presented label-free ratiometric fluorosensor based on CDs for the selective and sensitive detection of enteroviral RNA. By using CDs as a reference fluorophore, ethidium bromide (EB) as a specific fluorophore, and a single-stranded DNA fragment (Probe), it enabled detection of enteroviral RNA release in vitro through a charge transfer mechanism between CDs and EB. The charge transfer was enabled via covalent functionalization of CDs with Probe. In this Func sensor the Probe-functionalized CDs were mixed with EB while the Non-Func sensor included a mixture of unmodified CDs, Probe, and EB. Building on this previous work, we now aim to address the high toxicity of EB by replacing it with the less harmful SYBR Green, thus allowing in vivo experiments. Preliminary results so far support the hypothesis that the SYBR Green would maintain the sensitivity of the EB system, while offering a less toxic alternative for in situ detection.

One-Dimensional Atomic Chains of Elemental Metals

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Low-dimensional materials exhibit extraordinary properties that make them promising candidates for advanced technologies. Although they have been investigated extensively, most of the research has focused on layered two-dimensional materials. Here, inspired by recent advances in atomically thin metallenes, we further reduce dimensionality and use density functional theory simulations to study the geometry, energetics, elasticity, and electronic structure of 40 non-magnetic one-dimensional (1D) atomic chains of elemental metals. We find that nearly all chains have a buckled ground state, nine chains are distorted, and three chains—Cd, Hg, and Sr—are semiconducting with an electronic gap. We also find that transition metals retain a substantial fraction of their three-dimensional bulk cohesive energy even in 1D chains. We assessed chains' dynamical stabilities by molecular dynamics simulations and found that 26 of them are thermodynamically stable at 100 K. Given that experimental techniques have recently reached the 1D-chain limit, our systematic study provides a foundation and timely guide to accelerating synthesis and characterization of these materials.

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

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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 [3].

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Direct transfer to obtain PMMA-free graphene on flexible PDMS

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Obtaining clean high-quality graphene remains a persistent challenge within the graphene community, as the widely used PMMA assisted transfer method often introduces polymer residues that compromise device performance. Here, we present a spin-coating based novel method for PMMA-free, direct wet transfer approach to obtain clean high-quality CVD graphene on thin flexible PDMS films. We have successfully transferred monolayer graphene with an area of 25 mm².

AFM measurements confirm uniform graphene coverage with the absence of visible cracks or tears. The spatial intensity variation of the 2D Raman peak is within 20%, demonstrating intact graphene coverage. Raman peak positions of the G band, 2D band and the 2D vs G bands correlation suggest weak coupling between graphene and the PDMS substrate, with a small tensile strain. The narrow distribution of 2D FWHM, the high I_{2D} / I_G ratio and low I_D / I_G ratio confirms the high quality of the transferred monolayer graphene.

Optomechanical readout for dressed donor spin qubits in silicon

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Quantum computers have not yet reached their full potential as there is yet to be a high-fidelity large scale qubit platform. One possible qubit realization that could have the required properties are donor spins in silicon, as they combine long coherence times with industrially relevant fabrication methods. However, donor spins in silicon are at the moment lacking a scalable and convenient readout method. Optimally, these spin qubits would be read out optically, as it allows for higher temperature operation and direct integration into silicon photonics platforms.

Unfortunately, donor spins in silicon don't have an optical transition at usable wavelengths. This issue could be bypassed by coupling them to a mechanical mode, which would then allow measuring the spin-state optomechanically. Specifically, our work aims for coupling with a low-frequency (MHz) mechanical mode, which requires first dressing the donor spin transitions with a microwave drive.

This method has multiple advantages, such as the dressing decoupling the spin from low frequency noise, while using the mechanical mode to indirectly couple the spins and optics and possibly enabling also coupling multiple qubits simultaneously.

The spin-mechanical coupling can be achieved either via strain or a micromagnet induced magnetic field gradient, while the optomechanical coupling is achieved via a photonic crystal nanobeam structure.

This poster will present our progress on achieving coupling between dressed donor spins and the nanobeam resonators.

Functionalization of femtosecond laser processed graphene surface for neuroapplications

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Graphene is a promising material for neural interfaces due to its high electrical sensitivity, mechanical flexibility, and biocompatibility. Here, we explore graphene surface functionalization strategies that enable two complementary functionalities relevant to neural interfaces: neuronal guidance and neurotransmitter sensing.

For neuronal guidance, graphene surfaces were patterned using two-photon oxidation (2PO), a femtosecond laser-based technique that introduces oxygen-containing functional groups with micrometer-scale spatial control [1]. Subsequent functionalization with poly-D-lysine (PDL) resulted in selective adsorption on pristine graphene and anti-selective adsorption on oxidized regions. Atomic force microscopy (AFM) confirmed spatially controlled PDL deposition, demonstrating the potential of 2PO-patterned graphene to create guidance cues for directed neuronal growth. Ongoing work focuses on optimizing deposition selectivity and evaluating the ability of these patterned surfaces to guide axonal growth *in vitro*.

In a complementary study, graphene field-effect transistors (GFETs) were functionalized with nanodisc-embedded acetylcholine receptor proteins to enable selective neurotransmitter detection. AFM characterization verified the successful deposition of individual receptor-containing nanodiscs on graphene surface. Current studies are evaluating the sensing performance of these functionalized GFETs toward acetylcholine detection.

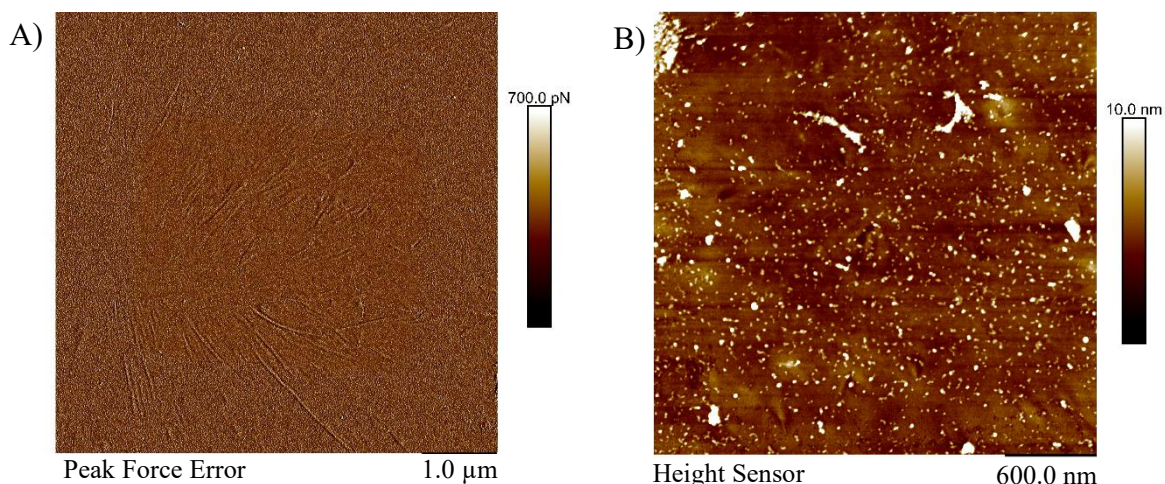


Figure 1: A) AFM image showing selective PDL deposition on pristine graphene with minimal deposition on oxidized region (3 x 3 μm square in the middle). B) Nanodisc-embedded acetylcholine receptor protein deposition on graphene surface.

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Quantum dots as charge sensors for donor spin readout

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Silicon is a promising platform for scalable quantum technologies due to its compatibility with existing semiconductor fabrication and its potential for integrating qubits, control electronics, and photonic components on a single chip. Among the various silicon-based qubit implementations, donor spins in silicon offer long coherence times and high control fidelities [1]. However, donor spin readout remains challenging with existing techniques. In this work, we explore the use of silicon quantum dots as charge sensors for donor spin readout.

The proposed readout scheme is based on a spin-selective donor-bound exciton transition under an applied magnetic field [2]. The exciton state relaxes via Auger recombination, leading to the ionization of the donor. This ionization can then be detected electrically using nearby quantum dots as charge sensors, enabling donor spin readout. To ensure scalability of the readout approach, we use gate defined silicon quantum dot devices developed by Semiqon Oy. These devices are fabricated on silicon-on-insulator platforms and incorporate on-chip multiplexing architectures, enabling the operation and characterization of multiple quantum dot structures on a single chip [3].

In this presentation, we will discuss the electrical characterization of these devices and evaluate their suitability as charge sensors for donor-based quantum systems. The devices, fabricated on silicon-on-insulator (SOI) platforms and equipped with on-chip multiplexers, enable control over multiple quantum dot devices on a single chip, making them well suited for large-scale quantum systems.

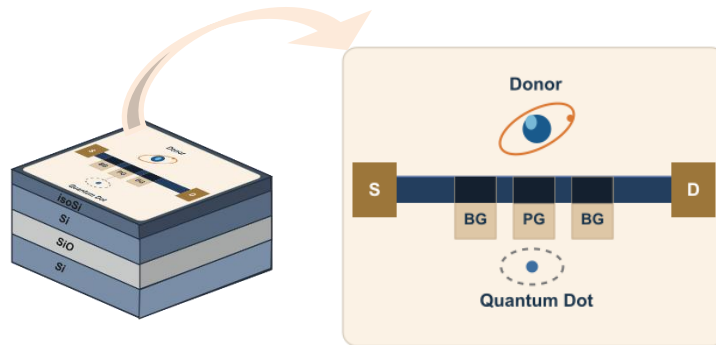


Figure 1: Schematic of the device with both donor and quantum dot on the same chip

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Introducing vibrational quantization in classical molecular dynamics under strong light-matter coupling

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Recent experiments have shown that vibrational strong coupling (VSC), a cavity quantum electrodynamics phenomenon, can alter chemical reactivity by changing kinetics, mechanisms, and product distributions.[1-4] VSC arises from the formation of hybrid light-matter states when molecular vibrations couple to photonic cavity modes, enabling modification of molecular wavefunctions without external illumination. While this possibility of controlling reactivity has generated major excitement, no predictive theoretical framework exists. Despite growing experimental evidence, it remains unclear when and how VSC affects reactions, posing a key fundamental challenge and limiting potential applications.

Our work aims to model VSC with atomistic details using a classical molecular dynamics (MD) approach. Since vibrational degrees of freedom are not quantized in classical mechanics, we propose to overcome that limitation by combining classical molecular mechanics (MM) or semi-classical quantum mechanics/molecular mechanics (QM/MM) potentials with a biasing potential, effectively imposing quantization on the relevant vibrational transitions in MD simulations. I will present benchmark results demonstrating the incorporation of vibrational quantization into classical MD simulations, first in the absence of an optical cavity and subsequently in its presence. These results demonstrate that the biasing potential successfully reproduces quantized vibrational behavior in an optical cavity. This methodology therefore provides a foundation for extending the approach to molecular systems under VSC, enabling future investigations of chemical reactivity under VSC conditions.

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Finite element estimation of nanoparticle-induced changes in cartilage mechanics

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Background: Cationic tantalum oxide nanoparticles (Ta₂O₅-cNPs) improve visualization of articular cartilage (AC) in contrast-enhanced computed tomography (CT) [1]. The Ta₂O₅-cNPs bind to negatively charged proteoglycans (PGs), reflecting specific cartilage compositional and biomechanical properties [2]. However, the effect of NPs on the biomechanical properties of AC remains unknown. **Methods:** Bovine osteochondral plugs ($n=30$, diam.=7 mm) were mechanically tested (Fig. 1A-B) before and after 93 h immersion in Ta₂O₅-cNP bath (30 mg/mL). Fibril-reinforced poroelastic finite element model was used (Fig. 1C) to estimate changes in non-fibrillar matrix modulus E_{nf} , initial fibril network modulus E_f^0 , strain-dependent fibril network modulus E_f^ϵ , initial permeability k_0 , and permeability strain-dependency factor M [3]. To quantify the extent and kinetics of NP uptake, an exponential model $[P(t)=P_{\max}(1-\exp(-t/\tau))]$, was fitted to the time-resolved μ CT data (Fig. 1E), where $P_{\max}$ represents the partition at the equilibrium and τ is the diffusion time constant. **Results:** Ta₂O₅-cNPs decreased E_{nf} by 47% and k_0 by 84%, consistent with cationic NP binding to negatively charged PGs and accumulation within the cartilage pore structure (Fig. 1D). In turn, τ correlated positively with pre-immersion E_{nf} and negatively with k_0 (Fig. 1E), suggesting that stiffer non-fibrillar matrix and lower initial permeability delay NP equilibration. **Conclusion:** Finite element modeling links NP uptake and retention to matrix- and fluid-related changes in cartilage mechanics, providing a framework for assessing the functional consequences of tissue retained NPs.

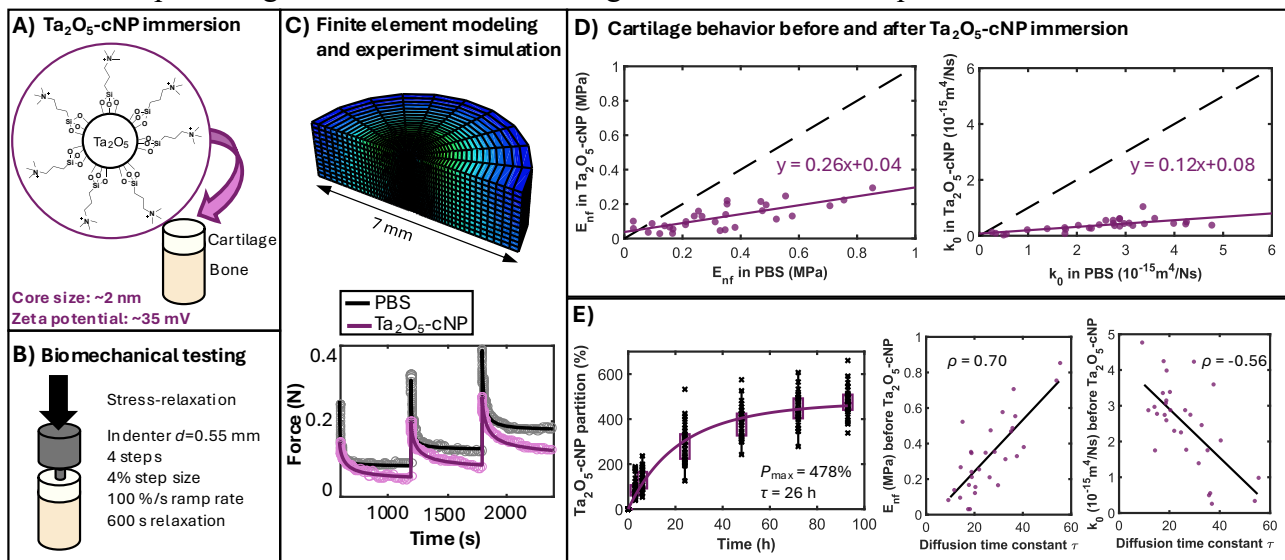


Figure 1: A) Ta₂O₅-cNPs were diffused into cartilage. B) Biomechanical stress-relaxation testing was conducted before and after Ta₂O₅-cNP immersion. C) Biomechanical testing was simulated with finite element modeling to estimate constituent-specific function of cartilage. D) Comparison of cartilage properties after Ta₂O₅-cNP immersion with baseline measurements in PBS of E_{nf} and k_0 . The dashed line represents the one-to-one ratio, and data points below it means decrease in the parameter after Ta₂O₅-cNP immersion. E) Ta₂O₅-cNP diffusion curve $[P(t)=P_{\max}(1-\exp(-t/\tau))]$, and Spearman correlations of τ with E_{nf} and k_0 .

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Area-selective ALD on high quality graphene

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The chemically inert nature of two-dimensional materials, particularly graphene, presents a significant challenge for the deposition of thin films using atomic layer deposition (ALD). To overcome this limitation, we employ direct femtosecond two-photon oxidation (2PO), a non-destructive and highly controllable method that locally functionalizes the graphene surface by introducing oxygen-containing groups, such as hydroxyl and epoxy species [1]. These functionalized regions act as effective nucleation sites for area-selective ALD, enabling the growth of uniform and ultrathin films [2,3]. Furthermore, our studies demonstrate that graphene coated with ALD-grown ZnO on oxidized regions can be restored to its pristine state through subsequent annealing [2]. In this work, we present our results on the selective deposition of ZnO, and its possible applications.

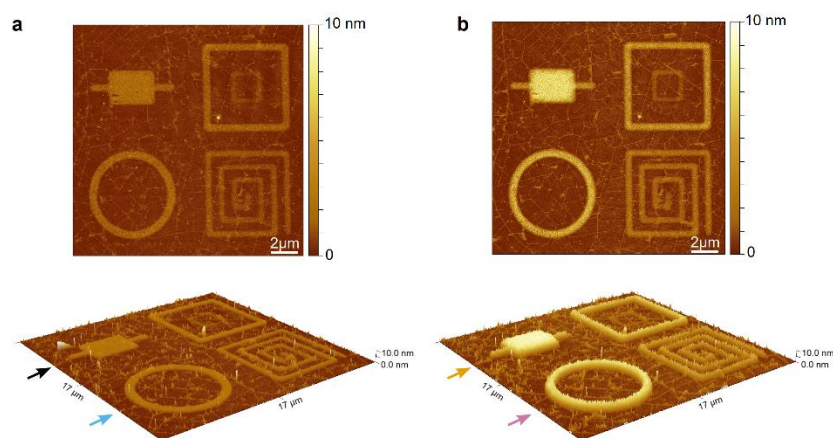


Fig 1: AFM images of (a) graphene after two-photon oxidation (2PO) and (b) after subsequent area-selective ALD [2].

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Role of central metal atom in electroluminescence induced energy transfer between phthalocyanine molecules

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Photosynthetic energy transfer between chlorophylls and carotenoids is essential for directing absorbed solar energy toward reaction centers, where it drives the production of chemical energy.

[1] Although the mechanisms underlying this energy transfer are well established at the macroscopic level, their quantum-mechanical properties remain incompletely understood. In particular, the influence of the central metal atom within the chlorophyll porphyrin ring on molecular excitation and energy transfer remains an important question.[1,2,3]

Here, we investigate the influence of the central metal atom on molecular optical properties and intermolecular energy transfer using metal-phthalocyanine (MPc) molecules as a model system. MPcs provide a stable and structurally well-defined analogue for chlorophyll, making them suitable for investigation with scanning tunneling microscopy (STM). Low-temperature, ultrahigh-vacuum STM-induced electroluminescence enables the optical properties of individual molecules and molecular dimers to be studied under controlled and reproducible conditions.[2,3]

We examine zinc (Zn), tin (Sn), and lead (Pb) phthalocyanine to investigate the effect of the central metal atom on the physical and optical properties of MPc molecules. Our results demonstrate a systematic redshift in the emission with increasing atomic mass of the central metal. In addition, heavier central metals introduce distinct optical characteristics and physical properties, including tunable molecular configurations associated with changes in emission and splitting of the emission peak.[3] These findings demonstrate that the central metal atom provides a means of controlling the optical response of MPc molecules and offer insight into the molecular-scale mechanisms governing energy transfer and emission in pigment-like systems.

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Strain-Mediated Coupling Between a Flip-Flop Qubit and a Mechanical Resonator

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Hybrid quantum systems combining spin qubits and mechanical resonators offer a promising platform for coherent control and quantum information processing. In this work, we study the coupling between a bismuth donor flip-flop qubit in silicon and a GHz-frequency mechanical resonator, arising from strain-induced modulation of the hyperfine interaction. This mechanism enables coherent spin-mechanical interactions in a solid-state setting.

We model the coupled system using a quantum master equation approach to capture both coherent dynamics and dissipative effects. We present results on mechanically induced shifts of the flip-flop qubit transition frequency, as well as coherent exchange dynamics between the flip-flop qubit and the mechanical mode. We further analyze how these effects depend on parameters such as detuning, coupling strength, and resonator occupation.

We also extend the model to multiple qubits and demonstrate how a coherently driven mechanical resonator can mediate interactions within a spin ensemble, enabling the exploration of collective dynamics and providing a possible route toward scalable hybrid quantum architectures.

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