

FROM SOLID STATE TO BIOPHYSYSICS XI

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UV and Blue Photophysics of Shallow Nitrogen-Vacancy Centers in Diamond

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Abstract

Photogenerated radical pairs (RPs) excited by UV and blue light play pivotal roles in biology involving, e.g., cell function, chemical transformations, and magnetoreception. Recently, RPs in artificial chemical architectures have also gained interest as building blocks for quantum information processing. Quantum sensing of RPs with the negatively charged nitrogen-vacancy (NV) center in diamond offers a new way to track the photogeneration of these paramagnetic species at the single- to few-molecule level, providing fresh insight into the spin evolution and complex reaction cascades involved.[1] Manipulated by light and microwave pulses, these singlespin sensors enable highly localized detection of nuclear and electron spin dynamics in molecules under ambient conditions with extreme magnetic field sensitivity. The experimental realization of such a sensor, however, requires understanding of the spin and ionization dynamics of shallow NV centers under UV and blue light irradiation. Here, we explore the effects of 375 nm and 445 nm excitation of shallow (ca. 10 nm deep) NV centers hosted in diamond nanopillar waveguides. Using green and orange lasers to initialize and read out the state of individual NV centers respectively, both spin and charge state of NVs are measured as a function of UV/blue laser power and pulse duration in pulsed optically detected magnetic resonance (ODMR) experiments. By systematically exploring this parameter space, we show both the capabilities and limitations of shallow NVs for probing photochemistry driven by UV and blue excitation for electron paramagnetic resonance spectroscopy and imaging at diamond surfaces.

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A Narrow Magic Window for Heavy Fermions near the Magic Angle in Twisted Bilayer Graphene

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Abstract

The notion of a single "magic angle" in twisted bilayer graphene has evolved into a fascinating array of magic angles and ranges each describing different facets of the material's behavior. While the original continuum model predicted a nominal magic angle, its simplicity ignored the intricate interplay of different physical phenomena. For example, lattice relaxation near the magic angle shifts its value upward, only to be counteracted by pseudomagnetic fields, that restore the original value. Including a symmetry allowed relaxation parameter changes this magic angle to a magic range. Yet another magic angle emerges from the coupling to phonons when the Fermi velocity equals the phonon sound velocity. Building upon this rich tapestry of magical effects, we will discuss our recent work on the convergence of lattice relaxation and Hartree interaction near the magic angle. We unveil a previously unreported Lifshitz transition to a Fermi surface topology that supports a "heavy fermion" pocket and an ultraflat band pinned to the Fermi energy. Analytical and numerical insights shed light on the narrow "magic angle range" where the "heavy fermion" is stable and make predictions for its experimental observation. We believe that the bands presented here are accurate at high temperature and provide a good starting point to understand the myriad of complex behaviour observed in this system.

Identification of cyanotoxins with a biological nanopore

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Abstract

Microcystins (MCs) are cyanotoxin oligopeptides produced by cyanobacteria, which strongly compromise water quality (1,2). Direct monitoring of cyanotoxin concentrations in water is challenging, mainly due to their low concentration in water and large structural diversity, impeding their identification (3,4). The limitations of the present analytical methods can be overcome by the development of a single-molecule nanopore-based sensing platform allowing for a portable, real-time, standard-free measurements for cyanotoxins in freshwater. This approach, relying on electrical signal detection, have shown the ability to discriminate already three different variants, although not at concentrations typically found in lakes and rivers (5). Here we used a different nanopore, which has shown to improve cyanotoxin detection and quantification, which is crucial for preserving water quality and protecting public health. We have been able to distinguish seven MC variants (differing by only one or two amino acids) based on their unique pore blockage characteristics. Additionally, we have shown that the discrimination of three main MC variants, when spiked into the lakewater matrix by using our technique, is feasible and could be used for the detection and discrimination of MCs.

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Low-noise nanopore in two-dimensional non-vander-Waals materials for single molecule sensing

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Abstract

Nanopores in ultra-thin membranes, particularly in two-dimensional (2D) configurations, offer exceptional sensitivity and precision for single-molecule biosensing. Nevertheless, their efficacy is hindered by significant 1/f noise when fashioned from typical van-der-Waals (vdW) 2D materials like graphene and MoS₂, posing challenges in achieving high-quality, low-noise 2D nanopores¹.

Two-dimensional metal oxide (MO) films, derived from non-vdW materials, exhibit distinctive electronic and chemical characteristics, rendering them promising substrates for 2D nanopore development. In this work, we introduce the fabrication of ultra-thin 2D metal oxide nanopores utilizing SnO_x and Ga_2O_3 membranes, with thicknesses ranging from 1 to 3 nm, achieved through an efficient and cost-effective liquid metal exfoliation method². Importantly, these nanopores demonstrate a 1/f noise profile significantly lower—by 2-3 orders of magnitude—than conventional 2D nanopores. Our investigations reveal that these 2D MO nanopores can effectively detect and analyze numerous individual DNA molecules, without undesirable interactions or unintentional reduction in DNA translocation speed. With their low noise levels and economically viable ambient-temperature fabrication process, 2D metal oxide nanopores emerge as a promising avenue for various single-molecule biosensing applications.

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Mechanistic-insight based controlled pore formation and scale-up of porous single-layer graphene membrane

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Abstract

Porous two-dimensional selective films where pores act as zero-dimensional aperture are highly attractive for rapid permeation of molecules where one can tune molecular transport, and therefore, molecular selectivity and flux by tuning pore size and pore edge functional groups. Porous single-layer graphene film is emerging as a highly attractive candidate to achieve ultrahigh flux given that it is just one atom thick, and that the scale-up of large area graphene by chemical vapor deposition is already successful. However, pore formation in graphene remains stochastic with trial-and-error approaches used for pore formation.

Controlled oxidative etching of graphene, e.g., using ozone, is highly attractive because one can decouple the events that leads to pore nucleation and growth. This allows one to control pore size by systematic oxidant exposure. I will discuss the series of events which takes place during oxidation ultimately yield a Å-scale pore. Briefly, this involves a cooperative assembly of epoxies which first forms cyclic epoxy trimers followed by linear chains of trimers, and finally an ordered honeycomb superstructure. The degree of order in these clusters is highly surprising mainly because oxidized graphene domains were once thought to be amorphous. Luckily, it is opening new avenues to control the pore size, e.g., by a controlled gasification of the cluster. The knowledge of edge functional group surrounding graphene pore, previously inaccessible by the microscopy studies, allows one to also carry out controlled functionalization of pore, e.g., to incorporate pyridinic N at the pore which remarkably improve the CO₂/N₂ separation performance of the pore. Thanks to the simplified chemistry of forming pores, and recent progress in crack-free transfer of graphene, A4-sheet-sized membranes can be prepared. Field trial of these membranes using industrial flue gas show highly promising results.

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Magnetism and band structure of a magnetic semiconductor

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Abstract

Europium cadmium arsenide, EuCd₂As₂, has emerged as a topological material where magnetism may produce strong effects. This compound has been understood as a candidate Weyl semimetal, based mostly on ab initio calculations, transport and photoemission measurements. I will present our recent results on samples in which we control the carrier concentration through chemical synthesis. We find magneto-optical evidence of a sizeable band gap, remarkably sensitive to the local Eu magnetism. Our results contradict the current consensus on the ground state of this compound, bringing into question its topological nature.

Towards nanopore protein sequencing

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Abstract

The nanopore sensing method holds the promise of delivering a single-molecule technology for identification of biological proteins, direct detection of post-translational modifications, and perhaps de novo determination of a protein's amino acid sequence. The key quantity measured in such nanopore sensing experiments is the magnitude of the ionic current passing through a nanopore blocked by a polypeptide chain. In contrast to DNA strand which carries a uniform negative charge regardless of its nucleotide sequence, capturing and keeping an unevenly charged peptide taut through the nanopore's constriction is a major challenge in nanopore sequencing of protein.

This talk will describe our latest progress in using molecular dynamics simulations to aid the development nanopore protein sequencing. The all-atom molecular dynamics method will be used to delineate the factors affecting the blockade current modulation by the peptide sequence [1]. The predictive power of the method will be demonstrated by uncovering the "sticky ion action" that transforms any biological or solid-state nanopore into a highly selective anion channel characterized by a giant electro-osmotic effect [2]. The talk will conclude with a description of our ongoing work to increase accuracy of coarse-grained simulations to reach the time scales of nanopore translocation experiment while preserving the accuracy of the all-atom method.

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Engineering Electrochemical AttoSens Platforms for microRNA Detection using Peptide Nucleic Acid Probe-functionalized 2D Nanomaterials

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Abstract

MicroRNA represents a class of short (~22 nucleotide) non-coding RNA, which hold great promise as 'liquid biopsy' biomarkers due to their gene regulatory functions and dysregulated patterns in many diseases including cancer. However, their short lengths and low circulating concentrations make them challenging to detect, even with gold-standard techniques like RTqPCR. There is thus an urgent need to develop simpler and more robust microRNA biosensors that offer high sensitivity and specificity while being amenable to point-of-care testing. In this talk, I will present two electrochemical biosensing platforms based on the rational design of 2D nanomaterials functionalized with bespoke Peptide Nucleic Acid (PNA) probes. While PNAs, which are synthetic pseudo-peptide analogues of DNA, offer greater stability, sequence specificity, and resistance to degradation compared to their natural counterparts, 2D nanomaterials like graphene and MXene offer attractive electrical and physicochemical properties.

Using the method of solid phase peptide synthesis, we have developed bespoke PNA probes with two types of functionalities, enabling either bio-orthogonal click chemistry or π - π stacking on the biosensing surface. Successful fabrication and biofunctionalization were validated through physicochemical and surface characterization techniques including XPS, XRD, and Raman spectroscopy. Both platforms demonstrated attomolar sensitivity (hence, 'AttoSens'), singlenucleotide specificity, and a wide dynamic range. Ultimately, this talk will demonstrate the immense potential of PNA-functionalized 2D nanomaterials in the development of ultrasensitive amplification-free point-of-care biosensors, enabling the next generation of minimally-invasive disease diagnostic technologies.



Figure 1. A smartphone-interfaced electrochemical biosensor based on laser-induced graphene with π - π stacked PNA probes enables ultrasensitive detection of microRNA biomarkers from serum

Nanofluidics in Fluctuating and Actively Driven Ultrathin Membranes

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Abstract

Transport in ultrathin membranes has gained significant attention over the last couple of decades. Thermal fluctuations in the membrane as well as externally driven mechanical deformations can be comparable to the critical dimensions of an ultrathin membrane. At this limit, transport of fluids through nanoporous membranes is not well understood. In this talk, we will investigate how atomic-scale vibrational coupling at a solid-fluid interface affects wettability and other fluid properties such as friction and slip. First, by performing all atom molecular dynamics (MD) simulations, we investigate how the wetting of water droplets on a substrate changes with the frequency of excitation of the substrate. We show that the wetting properties can be significantly altered by the frequency of excitation. We discuss the mechanisms governing physicochemical behavior of fluids at solid-fluid interfaces in the presence of vibrational coupling. Next, we investigate water and ion transport through confined spaces. We discuss the effect of wall excitations on friction coefficient and water and ion transport. We show that transport rates can be quite different from rigid counterparts. Finally, we investigate water transport through vibrating nanoporous membranes and show that non-equilibrium fluctuations can have a significant effect on water transport. We discuss some potential applications that could benefit from these studies.

Nanoelectrical characterization of clean energy materials

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Abstract

The need for efficient renewable energy solutions has never been more critical in the pursuit of a sustainable future. Beyond their impact on mitigating the environmental effects of conventional energy sources, such as fossil fuels, they will offer improved economic resilience and energy security.

The main catalyst for this transformation is the development of clean and cost-effective materials that are capable of harvesting renewable resources with maximum efficiency. However, the question remains as to which technological advances can accelerate the integration of these novel materials, from their development stage to their practical applications.

Clean energy materials often rely on reactive surfaces, enabling crucial interactions such as the efficient conversion of sunlight into electricity in photovoltaic materials [1] or facilitating chemical reactions for clean fuel conversion in fuel cells [2]. A complete understanding of their electrical, mechanical, morphological, and chemical properties at the nanoscale is essential for their development.

At the Dansk Fundamental Metrologi (DFM), Danish National Metrology Institute, we uphold the principles of precision and traceability within several key measurement areas, including nanometrology. With our expertise in nanocharacterization, including scanning electron microscopy (SEM), atomic force microscopy (AFM), and Kelvin probe microscopy (KPFM), we extract in-depth information about nanomaterials. Using metrological methods, we offer direct quality control throughout the material development process and for future renewable energy devices.

In this study, we demonstrate the application of conductive AFM and KPFM to novel clean energy materials under diverse ambient conditions. Metal oxide layers will be tested for UV-enhanced photocatalysis, offering a new solution for hydrogen production, ultimately eliminating the need for rare elements. Additionally, hybrid halide perovskite, a potential game changer in the solar cell industry [3], will be tested in controlled environments (humidity, temperature, and electric field) to explain the role of defects in their unique ability to self-heal.

Through the optimization of these nanoelectrical characterization techniques by allowing external influences in situ, we aim to offer new avenues for the exploration of materials for renewable energy applications, thereby facilitating an even faster transition to a green future.

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Nanopore microscopy for single-cell protein profiling

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Abstract

Nanopore sensors are used as a tool for quantifying protein levels in biological samples, yet significant challenges hinder their application in protein detection in live cells. These obstacles include the need for portability to enable sensor placement within or near live cells, the requirement for precise in situ control of pore size, and the necessity for improved specificity to identify proteins while minimizing non-specific interactions with the pore. We aim to address these challenges by advancing nanopore microscopy for single-cell profiling, and to explore its potential in cell biology applications.

In this presentation I introduce the concept of interface nanopores,^{1,2} and how these nanopores act as microscopic windows, allowing for real-time monitoring and analysis of cellular processes such as protein secretion. Our aim is to further develop this methodology for single-cell proteome and secretome profiling. Specifically, we aim to investigate the mechanisms underlying antibody production and secretion in B cells, as well as elucidating the dynamics of protein secretion during the interaction of (CAR-) T cells with cancer cells. By tackling these challenges and expanding the capabilities of nanopore microscopy, we seek to pave the way for the transformative applications of nanopore sensors in single-cell biology and immunology studies.

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Gate tunable spin transport in a two-dimensional semiconductor

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Abstract

Exploitation of the intrinsic spin of an electron, spintronics, facilitates the development of multifunctional and novel devices which could play an important role in the Beyond-CMOS era. Two-dimensional (2D) crystals and their van der Waals heterostructures are particularly promising for spintronics device applications due to their unique properties, including strong responses to field effect gating and proximity interactions, which may enable new functionalities that are not possible with conventional bulk materials [1].

Black phosphorus is a particularly promising 2D semiconducting material for spintronics research due to its high charge mobilities, low atomic mass, and puckered crystalline structure, which are expected to lead to anisotropic spin transport with nanosecond spin-lifetimes. In this seminar, I will introduce ultra-thin BP as a unique platform for studying rich spin-dependent physics. Firstly, I will show that BP supports all electrical spin injection, transport, precession and detection up to room temperature [2]. Then, I will present our recent findings on the impact of the unique crystal structure of BP on its spin dynamics, revealing strong anisotropic spin transport along three orthogonal axes [3]. The exceptional spin transport and its strong gate-tunability together with the strong spin-lifetime anisotropy we observe in BP add to the growing body of evidence for the potential of 2D materials in functional spin-based device applications.

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Instantons within the Functional renormalization group

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Abstract

As spatial dimensionality gets lower it becomes more difficult for a system to order. At some dimensionality, the so called lower critical dimension, the fluctuations prevent ordering all together and the only way to order is to put temperature to 0. We discuss the scenario of the approach to lower critical dimension within the Functional renormalization group (FRG) for the scalar 4 theory. There we expect localized, instanton-like (kink-like) excitations to proliferate and the fixed point to disappear.

Despite FRG seemingly being a correct tool for the job, capturing this scenario has proven to be a difficult problem and one typically obtains the possibility of ordering where it should not be possible [1,2]. We uncover the analytical structure of the FRG that allows us to understand the source of the problem [3]. Remarkably we indeed find that FRG captures the localized instantonic excitations, albeit in a rather indirect way.

We shall discuss the applications of our work to some open problems that we believe we can elucidate, for example: a) quantum mechanical tunneling problem in the low temperature limit which appears in description of the Sine-Gordon problem [4]; b) the question of lower critical dimension in hysteresis [5].

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Interface-driven triplet proximity effects and electronic transport in spin-orbit coupled superconductor/ferromagnet hybrids

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Abstract

Superconductor/ferromagnet (S/F) hybrids, especially with spin-orbit coupling, provide an excellent platform to study several interesting phenomena ranging from spin triplet to topological superconductivity and the diode effect. These discoveries provide a platform for a wide range of applications in quantum technologies, some of which we have just started to explore [1,2].

In this talk, I will discuss recent theoretical and experimental progress in S/F structures which incorporate spin-orbit coupling in the context of spin triplet superconductivity. I will highlight our recent work where interface modification leads to a large triplet proximity effect [3] and some results on transport properties of these hybrid structures.

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Conjugated Oligoelectrolytes: A Versatile Platform for Membrane Modifications

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Abstract

Conjugated oligoelectrolytes (COEs) are a class of synthetic molecules characterized by a linear pi-conjugated segment and terminal ionic functionalities. The distribution of hydrophobic content and hydrophilic charged groups leads to spontaneous self-assembly within lipid bilayer membranes. One can observe subsequent modification of membrane properties that correlate to the structural features of the COE. Extended molecular lengths enable rigidification of the membrane and are largely non-cytotoxic. As such, one can design molecular probes with a range of optical features for bioimaging and, in particular, the characterization of nano-scale extracellular vesicles. Specific probes for flow cell cytometry of exosomes can be therefore designed, which offer advantages over commercially available dyes. By incorporating internal molecular rotors that modulate the rates of non-radiative emission decay rates, COEs can be prepared that can be used to image the membrane composition and tension in living cells, particularly as a result of environmental conditions or pharmacological treatment. Once inside the cells, the ratio of aromatic and charged groups determines intracellular distribution. This feature can be used to image the entire exocytic process (COE-S5) or as a tool to determine mitochondrial dysfunction (COE-CN).



Functional insights and novel applications in peptide discrimination and sequencing using the aerolysin protein pore

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Abstract

The pore formed by the bacterial toxin aerolysin is particularly suited for differentiation of single molecules by careful measurement of the ionic conductance remaining when they partially block the pore. This residual conductance has been shown not only to measurably vary with size (volume)¹⁻⁵ but also with the shape of the molecule, as shown by the differentiation of structural and positional isomers^{2,6}.

As we show using high-resolution/bandwidth measurements of resistive pulses in wtaerolysin and several variants produced by site-directed mutagenesis, this high sensitivity is due to an efficient molecular trap realized in the pore's beta barrel. Using these variants, we validate a kinetic four state model where analytes are being held for prolonged times in an energy minimum between two energy barriers that are largely formed by rings of charged (and bulky) amino acids at the beginning and the end of the pore's beta barrel. Importantly, in addition to facilitating polymer characterization, this trap affords the opportunity to follow single particle electrodiffusion in real time by electrical recording. We also show evidence for an asymmetric action of the second, *trans*-ward barrier, preventing access even for small, neutral analytes.

In addition, we show further evidence of (position-dependent) differentiation of very subtle chemical modifications such as histone protein citrullination and deamidation, where the changes in volume or molecular shape brought about by additive modifications such as acetylation and methylation, are absent or negligible and non-steric effects are paramount. These latter findings suggest that, at the limit of resolution, the current through the aerolysin pore might actually be sensitive to the electronic structure of a molecule.

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Microstructure-Dependent Optical Properties of Doped Spinel Oxide Nanosystems

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Abstract

Doped spinel crystals, with their unique luminescent properties in the visible and nearinfrared spectra, offer a world of possibilities. Excited by X-ray or UV-visible light, these crystals can be used in a variety of applications, from X-ray-mediated bioimaging and optical sensing to photodynamic therapy, as well as for security purposes in both civil and military sectors, such as anti-counterfeit technologies can benefit from the complex time-dependent optical properties of this material. Indeed, the different photoemission spectra upon X-ray or lower energy photons and the long-lasting luminescence, which involves prolonged emission due to trapped states and can last for hours, offer significant utility both separately and collectively. However, defect environment and crystal field strength around the dopant significantly influence the luminescent properties. Annealing processes, by modifying the electron trap states and defect structures within the crystals, can further impact their optical characteristics.

Our research has demonstrated that annealing hydrothermally synthesized spinel nanoparticles at low temperatures reduces the crystal field strength, resulting in a temperature-sensitive, quasi-melted pseudocrystalline surface[1]. This alteration leads to a noticeable decline in photon output and produces an emission that is both red-shifted and temperature-dependent. By meticulously optimizing the annealing conditions, we can significantly enhance the photoemission intensity or prolong the duration of LLP. Specifically, the emission spectrum of chromium-doped ZnGa₂O₄ can be aligned with the absorption spectrum of the photoimmunotherapy dye IR700. This alignment, facilitated by optimization, allows the activation of the anticancer agent using common X-ray sources such as CT scanners[2]. Consequently, this approach holds promising potential for treating deeply located or internal tumors and other medical conditions, heralding a new era in the combination of photodynamic-and photoimmunotherapies and medical imaging techniques.

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Vibrational and non-local elastic properties of amorphous media

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Abstract

Amorphous materials, such as glasses, amorphous polymers, biopolymers, and their nanocomposites, play an important role in various fields of science and technology. Such materials have a disordered arrangement of atoms and monomers, which leads to their unique thermal, elastic and vibrational properties. Understanding their properties is a key challenge in condensed matter physics, which aims to establish the link between macroscopic behavior and microscopic properties.

Due to the presence of disorder, only a small part of the low-frequency phonons in amorphous solids have a mean free path greater than the wavelength. The majority of vibrational excitations do not satisfy such an Ioffe-Regel criterion, but these vibrations are able to transfer energy by diffusion [1]. At the same time, an excess in the vibrational density of states, known as the boson peak, was observed near the Ioffe-Regel crossover in a number of experiments [2].

In addition, the heterogeneity length scale in amorphous solids significantly exceeds interatomic distances. At such length scales, the continuum theory of elasticity cannot be applied, which does not allow the description of composite systems containing nanometer-sized inclusions. At the same time, the addition of nanoparticles, which affects the microscopic behavior of a medium, can significantly change its macroscopic properties.

We have shown that the cooperative effect of strong disorder and the mechanical stability criterion makes it possible to apply the random matrix theory and provide a consistent theory of the vibrational and elastic properties of strongly disordered media. On the one hand, it explains the boson peak, the Ioffe-Regel crossover and the diffusion of vibrational excitations [3]. On the other hand, it gives constitutive equations for the elastic properties of a medium with arbitrary strong disorder [4]. In particular, it is shown that the formation of the interphase with increased stiffness around nanoparticles can be considered as a non-local disorder-induced effect [4,5].

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Non-adiabatic Lifshitz transition in High T_c superconductor Bi₂Sr₂CaCu₂O_{8+δ}

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Abstract

The equilibrium tunning of doping generates substantial changes in the electronic states of cuprates. They undergo a gradual transition from Mott insulator to Fermi liquid, crossing d-wave superconductivity. Usually, these changes are accompanied by an abrupt transformation in Fermi surface topology, the so-called Lifshitz transition. Here in this work, we address the effect of ultrashort pulses on the Fermi surface topology of cuprates $Bi_2 Sr_2 CaCu_2 O_{8+\delta}$ by means of time-resolved-Angle resolved Photoemission Spectroscopy with pump energy of 1.55 eV. For the first time, we demonstrate that high fluence pulses are significantly efficient in supplying the Fermi level with additional carriers through the photodoping process, driving non-adiabatically the Fermi surface from hole-like to electron-like.

Collective modes in electron systems: effects of Coulomb interaction and dimensionality

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Abstract

Collective modes have been intensively explored in a variety of two-dimensional materials and three-dimensional topological Dirac and Weyl semimetals. We present our recent results on collective mode spectra in topological nodal line semimetal and composite metal-monolayer semiconductor systems. Collective modes can be obtained by evaluating the dielectric function comprising the effects of Coulomb electron-electron interaction within the random phase approximation (RPA), and the energy-loss function that reveals their spectral weights and the influence of the electron-hole excitations.

We study the plasmon collective mode of a three-dimensional topological nodal line semimetal with two-dimensional Dirac electron energy bands crossing at the dispersive nodal line and the long-range three-dimensional Coulomb electron-electron interaction. We show that the anisotropic optical plasmon mode is damped entering the interband electron-hole continuum [1].

The Coulomb electron-electron interaction can be further screened in composite systems. We address the influence of a semiconducting monolayer of molybdenum disulfide (MoS_2) and tungsten disulfide (WS_2) on the plasmon mode of a supporting three-dimensional metal. The direct band gap in electronic structure and polarizability of monolayer MoS_2 and WS_2 give the interband dipolar mode, which couples to the intraband optical plasmon mode of the metal [2]. The hybridized modes have the polarization properties of the semiconducting monolayer and the supporting metal. We show that the coupled plasmon-dipolar modes are separated and that their spectral weights are comparable. The coupled plasmon-dipolar modes could be found in the composite systems with metallic oxide SrNbO₃ as metal.

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Through the pupil: What we can learn from the retinal vasculature about health and genes

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Abstract

Background/Objectives: Colour fundus images (CFIs) allow for non-invasive assessment of the retinal features providing important information on health. We recently characterised CFIs of 72k UK Biobank participants in terms of 17 tangible vascular traits (TVTs), many of which are routinely observed by ophthalmologists, such as vessel density, diameter or tortuosity, and showed that these phenotypes are modulated genetically and often associate with cardiovascular diseases or their risk factors [1,2]. We expand this analysis in terms of "deep" retinal features (DRFs) corresponding to latent space embeddings extracted from self-supervised deep learning models. Our objective was to quantify their phenotypic and genetic correlation to our TVT, heritability, and (added) value for disease prediction.

Methods: We applied the recently published RetFound model to data from the UKBB extracting 1024 DRFs both from CFIs and segmented CFIs showing only the vasculature. We performed GWAS on these two sets of DRFs, as well as their 17 leading principle components. We used simple Pearson correlation analysis and LD score cross trait regression to quantify phenotypic and genotypic correlations between TVTs and DRFs. We used linear and logistic regression, as well as Cox models to explore DRF disease associations and compare them to those of TVTs.

Results: Our analysis revealed that TVTs and DRFs provide overlapping but not redundant characteristics of CFIs. DRFs present a spectrum of heritability up to 17%, which is substantially lower than that of tortuosity (25%), which is however close to that of one of the leading DRF PCs. TVTs show stronger association than DRFs with systemic cardiovascular diseases such as stroke and myocardial infarction, as well as age at death, while the opposite was seen for diabetes and cataracts.

Conclusion: We conclude that TVTs and DRFs provide complementary characterisations of CFIs calling for more integrative methods to maximise their potential for early disease diagnosis and advancing our understanding of disease mechanisms through genetics.

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Nonlinear Tools for Deeper and Faster Bioimaging

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Abstract

Multiphoton excited fluorescence is just one facet of the multiple signals that arise from the nonlinear optical interaction between light and matter.¹ The acquisition of most of these nonlinear signals for microscopy applications has been hindered so far by a combination of technological limitations (such as a lack of suitable optical components) and sample-related challenges (particularly the photostability of biological samples exposed to high peak power irradiation). The recent availability of rugged femtosecond optical parametric amplifiers (OPAs) and optical parametric oscillators (OPOs) operating in the Short-Wave InfraRed region (SWIR, 1-2 μ m), along with picosecond Fourier Domain Mode Locked (FDML) lasers have disclosed exciting new possibilities for bioimaging, offering improved penetration depth and enabling fast volumetric imaging with minimal sample preparation requirements.



Figure 1. Multiphoton microscopy images of a live zebrafish upon SWIR excitation (1650 nm). Left: THG; Right: Blue: THG; red: SHG; green: 3-photon excited autofluorescence; scalebar 90 μm.

We will present results from our work combining second and third harmonic (SHG, THG) imaging, along with diffractive scanning for cell detection in tissues and biological fluids. Additionally, we will show how dielectric nanoparticles enhance the nonlinear response and can be used to significantly boost the speed of volumetric data acquisition.³ In conclusion, we will discuss the challenges associated with these imaging conditions in terms of sample photostability.

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Nodal-line resonance and its control by magnetic field in Co₃Sn₂S₂

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Abstract

Recently, the topology of the electronic band structure has attracted much attention in materials with broken time-reversal symmetry as these compounds may host non-trivial features such as Weyl fermion. The magnetic order may give rise to large anomalous Hall effect (AHE) in these compounds, which is a fingerprint of the non-trivial topology. Furthermore, magnetic fields may allow also the control of these peculiar band structure features. However, the experimental verification of these appealing ideas is challenging. Traditional magnetotransport experiments struggle to pinpoint the specific band features responsible for the AHE since it measures an integrated response of multiple bands combined with extrinsic contributions as well. Identifying the magnetic field-induced changes is also difficult in these multi-band materials.

Here, we highlight the power of magneto-optical methods in addressing these limitations. Using the archetypical topological magnet $Co_3Sn_2S_2$ as a model system, we demonstrate how measurement of the Hall conductivity spectrum allows for the disentanglement of the various contributions to the AHE [1]. We deduced all components of the conductivity tensor in $Co_3Sn_2S_2$ by measuring the polarized reflectivity as well as the magneto-optical Kerr-effect (MOKE) spectrum. A key observation was a resonant enhancement of the Hall conductivity at 40 meV, which primarily determines the static AHE, thus confirms its intrinsic origin. Our material-specific theory reproducing the experimental data remarkably well showed that the nodal lines gapped by spin-orbit coupling generate large hotspots of Hall spectral weight, while the Weyl points only give vanishing contributions. We further observed a significant enhancement of the linear dichroism at the nodal line resonance, suggesting to a new signature of topological states.

We also explored the impact of magnetic field direction on the optical conductivity of $Co_3Sn_2S_2$. By rotating the magnetization from out-of- to in-plane direction, we observed a reconstruction of the optical conductivity [2]. Our DFT calculations suggested that the in-plane magnetization leads to a reduction of the spin-orbit gap and change the band topology as well.

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Single atom magnets and single atom qubits

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Abstract

In his talk *There's Plenty of Room at the Bottom*, given at the APS meeting in 1959, Richard Feynman expressed the vision to ultimately store information in single atoms. The feasibility of magnetic information storage in single atoms has indeed been demonstrated in 2016, where two adsorbate/substrate systems with stable magnetic quantum states were identified [1,2]. These systems were labelled *single atom magnets* since each of these surface adsorbed single atoms behaves as a classical permanent magnet. The atoms can be magnetized up or down and remain in that state for hours. These results were confirmed by individually addressing these atom [3,4] and several further systems discovered that exhibit these fascinating properties [5,6]. The temperature at which the magnetization spontaneously relaxes is referred to as energy relaxation time T_1 (for the best systems it is infinite at 4 K and a few minutes at 45 K).

The next goal is to explore whether *single atom quantum bits* are feasible. This requires longlived magnetic superposition states that can be manipulated by external stimuli. One figure of merit of a qubit is its coherence time T_2 with respect to the Rabi period that quantifies how many operations can be performed until the state decays. Encouraged by lanthanide atoms in bulk insulators having long T_2 [7], we performed electron spin resonance measurements on single lanthanide atoms adsorbed at surfaces, which is the first step to understand nuclear and electron spin coherence in such systems [8].

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Single-molecule detection with low-noise solidstate nanopore

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Abstract

Recent progress in nanodevices has provided new opportunities in single-molecule detection, which is significant as it can not only transform the understanding towards biology by bypassing the ensemble averaged behavior and providing direct information on single molecule, and also enables variable clinic applications like early-stage diagnostics. Solid-state nanopore is a kind among such nanodevices, which has received intensive attention due to its high sensitivity, high device robustness and capability of integration with semiconductor industry to realize highthroughput detection, etc. However, although solid-state nanopores have been studied for various biomolecule detection applications, the sensing accuracy still remains a challenge due to, for example, the higher noise that can degrade the signal-to-noise ratio, and the fast translocation speed of biomolecule, thus hindering practical applications where an accurate sensing of biomolecule with dominant signal and sufficient temporal resolution are required. Therefore, in this work, we presented first a wafer-scale fabrication protocol of solid-state nanopores with lownoise characteristics, with which we are able to reach higher measuring bandwidth up to 10 MHz. Then we demonstrated the ability to detect ultrafast translocation of individual motif on DNA and single protein molecule on sub-microseconds timescale. The improvement here makes it promising to probe biomolecule dynamics at a much smaller time scale and also broaden the range of analytes that are clinically important but unable to be detected due to the limited resolution.

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Single molecule analysis of protein–lipid interactions in membrane

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Abstract

Proteins are the major building blocks of life, dictating most biological processes and cellular functions. Among these, approximately one-third of human proteins are membrane proteins, and around 60% of drug target proteins are located at the cell surface. Therefore, it is vital to monitor these membrane associated proteins interaction with lipids. Single-molecule techniques offer unparalleled sensitivity and the potential for extensive parallelization, making them promising tools for probing such interactions. Here, by using a high throughput lipid membrane platform, together with a second harmonic scattering measurement, we can quantitatively characterize the affinity of pore-forming proteins and lipids [1]. In addition, we showed that in vitro, that Turandot A (an a priori soluble protein from Drosophila) can bind phosphatidylserine lipid headgroups on membranes and inhibit the pore-forming activity of some antimicrobial peptides on eukaryotic cells [2]. Furthermore, we used our in vitro nanopore single-molecule system to mimic the in vivo transmembrane transport of proteins, and our results provide direct evidence supporting the entropic pulling mechanism of Hsp70s molecular chaperones which are central components of the cellular network [3]. Our results provide the details of protein-lipid interactions at the molecular level, offering a deeper understanding of membrane biology and facilitating the development of targeted therapeutics.

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Exploring mRNA Technology: Challenges and Opportunities for Physicists and Biophysicists

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Abstract

Moderna's mRNA technology has made a significant global impact, most notably through the Spikevax COVID-19 vaccine, and the technology continues to show promise across our development pipeline. This presentation will provide a concise overview of our mRNA platform, explaining how various components and processes integrate to produce effective mRNA-based medicines. Additionally, I will address some unique challenges in characterizing these systems and will highlight opportunities for physicists and biophysicists to develop advanced tools and techniques for the future advancement of mRNA technology.

Super-Structures in nickelate parent compounds

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Abstract

This talk will present synchrotron experiments on nickelates. Higher order magnetic interactions in La_2NiO_4 – reached through resonant inelastic x-ray scattering - will be presented. In a second part, oxygen structures of topotactically reduced Ni-113 nickelates will be discussed.

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Detecting the spread of Wannier functions and quantum geometry by optical sum rules

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Abstract

The spread of valence band Wannier functions in semiconductors and insulators gives a rough estimation of how insulating is the material, and is an important quantity in first-principle calculations. We elaborate that the gauge-invariant part of the spread can be extracted experimentally from optical sum rules, owing to the fact that it is equivalently the quantum metric of the valence band states integrated over momentum. Because the quantum metric is the matrix element of optical absorption, this implies that the spread in 3D materials can be obtained from the frequency-integration of the imaginary part of the dielectric function, and hence the dielectric function acts like a spectral function of the spread, as demonstrated for common semiconductors like Si. In 2D materials, the spread is given by the absorbance divided by frequency and then integrate over frequency. Applying this method to graphene reveals the importance of intrinsic spin-orbit coupling in obtaining a finite spread, and in twisted bilayer graphene we show that the absorbance can be used to estimate the spread of effective Wannier orbitals on the moire scale. Finally, we apply our method to hexagonal transition metal dichalcogenides to estimate the spread in these materials.



Figure 1: (top to bottom) Band structure, quantum metric, fidelity number spectral function, and absorbance of twisted bilayer graphene at five selected twisting angles.

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Realization of basic types of Andreev-molecules

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Abstract

Topological superconductivity provides a promising platform to realize fault tolerant quantum hardware. The simplest topological superconducting system is the Kitaev-model, which is a chain of localized sites where neighboring ones are coupled by superconducting pairing and direct tunneling. Since state-of-the-art semiconducting nanostructures allows to create artificial atoms and tunnel couple them or interconnect by superconductors, the basic ingredients are available to build up artificial chains, which we call superconducting artificial molecules, or Andreev-molecules. Very recently various realizations of such chains have been reported where the sites are coupled in different ways, e.g. via superconducting vacuum, superconducting bound state, or superconducting artificial atom.

We will present experimental realization of two types of Andreev-molecules: i) the analog of H_2 molecule, where two artificial atoms are tunnel coupled via a superconducting vacuum [1] and ii) the analog of H_20 molecule, where two artificial atoms are coupled via a 3rd superconducting atom [2].



Figure 1. Realization of different Andreev-molecules Left H₂ type, right H₂O type ones.

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Charge transport in organic conductors and manganites: Evidence for Mott-Anderson localization

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Abstract

One of the most fascinating aspects of condensed matter is its ability to conduct electricity, which stems from a strong tendency of valence electrons to delocalize in a periodic potential created by ions in the crystal lattice of a given material. In many advanced materials, however, this basic delocalization process competes with various processes that tend to localize these very same valence electrons, thus driving the insulating behavior. The two such most important processes are the Mott localization, driven by strong correlation effects among the valence electrons, and the Anderson localization, driven by the interaction of the valence electrons with a strong disorder potential. These two localization processes are in the literature almost exclusively considered separately from both an experimental and a theoretical standpoint.

Here we present an overview of our long-standing research on selected organic conductors [1-3] and manganites [4,5] that clearly show the presence of both these localization processes. The most important aspects are the presence of hopping transport and a counter-intuitive increase in conductivity with increase in disorder, observed in all studied materials. We argue that such behavior implies the localization of conducting charge carriers driven by the combined effects of correlations and disorder, which can be understood only within very rarely considered theories of Mott–Anderson localization. The basic idea is that the correlations open an energy gap at the Fermi level, thus promoting the insulating behavior, while the disorder fills in the gap with localized states at the Fermi level, thus increasing conductivity [6]. We believe that such behavior might be found in other related strongly correlated systems as well, and therefore be a generic feature of many advanced materials.

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Cell-mimicking nanolipogel for the control of biomolecules delivery

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Abstract

High initial burst release of biomolecules is just one of the many challenges faced by lipid based nanoparticulate formulations, even though it is widely used for drug encapsulation and delivery studies. One of the emerging potential strategies is the use of nanolipogels (NLG) to encapsulate drugs, which can suppress the initial burst release. However, current works are short on characterization of the mechanism for the release from NLG systems. Therefore, varying molecular weight of Poly (ethylene glycol) Diacrylate (PEGDA) in NLG were used to study the mechanism of release. To provide a further mechanistic study and characterization of the diffusion, a novel cell derived microlipogels system was developed. This solution was to overcome the limitations of Fluorescence Recovery after Photobleaching (FRAP).

Results has shown that different Mw of PEGDA gave different suppression of the initial burst release. FRAP results then gave further validation by showing that the smaller mesh size restricted the diffusion consequential of a lower mobile fraction. These gave clear insight into the possibility of controlling the encapsulation and release of biomolecules, by targeting the fabrication of nanogel core. From this, Chitosan Methacrylate NLGs was then studied to expand into other ways in manipulating the nanogel core for greater control. This design of NLG systems will allow the encapsulation of negatively charge biomolecules like siRNA. To study cell membrane coating of NLG, we developed of a novel Chitosan Methacrylate-Tripolyphosphate core, which allows the co-extrusion with cell membrane or extracellular vesicles. This opens the possibilities of using a multitude of cells and means the transfer of a multitude of different properties onto NLGs like exosomes membranes. All in all, it was shown that cell mimicking NLG system was able to provide a controlled release of biomolecules. Relationships with changes to the nanogel core as well as membrane coatings were also explored and proven to be viable and plausible expansions to other membrane origins.

This work, hence, provide a guide for designing NLGs to meet the needs of different clinical applications and drug delivery systems.

Single-molecule sensing with aerolysin poreforming toxins

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Abstract

Evolution has found countless ways to transport material across cells and cellular compartments separated by membranes. Protein assemblies are the cornerstone for the formation of channels and pores that enable this regulated passage of molecules in and out of cells, contributing to maintaining most of the fundamental processes that sustain living organisms. As in several other occasions, we have borrowed from the natural properties of these biological systems to push technology forward and have been able to hijack these nano-scale proteinaceous pores to learn about the physical and chemical features of molecules passing through them [1].



Using integrative structural biology, i.e. combining molecular modeling and simulations along with biochemical and cryo-EM analysis, we have revealed the structure and assembly mechanism of one of the most studied bacterial pore-forming toxins [2], namely aerolysin from *A. hydrophila* [3,4], recently obtaining its highest resolution structure at 2 Å by cryo-EM in nanodiscs (unpublished). Leveraging this structural and functional understanding, we have been able to characterize its properties as a molecular sensing device that can accurately discriminate nucleic acids and peptides [5], as well as detect post-translational modifications associated with validated biomarkers of neurodegenerative diseases (e.g. a-synuclein phosphorylation in Parkinson's disease)[6]. Moreover, we have explored the ability of aerolysin pores to decode the information stored in hybrid polymers with the aim of finding new, alternative solutions for the emerging problem of data storage [7]. We are further leveraging and engineering the exquisite sensitivity of aerolysin pores as well other biological pores from the same superfamily to develop the next generation of sensor devices for single-molecule proteomics and analytical chemistry.

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Pushing the limits of membrane selectivity in nanoscale transport channels

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Abstract

Separations of solutes in water flowing through 1D and 2D confined networks provides a platform for systematically studying transport under nanoscale confinement. For 2D confinement, a method to tune spacing and chemical environment of the interlayers in membranes comprised of phyllosilicate materials is presented [1,2]. By employing alkanediamine crosslinkers, the interlayer galleries' height can be controlled, and these systems display enhanced membrane stability and tunable ion separations. For 1D transport, the potential of near-perfect isoporous membranes combined with process engineering is offered as a route to overcoming traditional limitations of solute rejection mechanisms [3]. This advancement suggests new opportunities for unprecedented membrane separations through careful process design and tight pore-size distributions.

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2D Quantum Materials for Spin-based Logic and Memory Devices

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Abstract

Two-dimensional (2D) materials represent a new platform for realizing novel quantum and spin-based phenomena and device applications. Engineering 2D heterostructures by combining the best of different materials in one ultimate unit can offer a plethora of opportunities in condensed matter physics. While materials such as graphene are suitable for spin-polarized electron transport, magnets and materials with topological spin textures are useful for spin-polarized electron sources. We utilized large-area CVD graphene for spin interconnect and realized multifunctional spin logic operations at room temperature [1,2]. To generate spin polarization and their electrical control, we engineered 2D material heterostructures by combining the 2D semiconductors [3], topological insulators [4,5] and magnetic materials [6] with graphene to realize strong proximity-induced spin-orbit coupling and magnetism in graphene.

Furthermore, nontrivial topology in the electronic band structure of quantum materials also makes them potential candidates for emerging technologies. We showed that their unique band structure and lower crystal symmetries can provide an unconventional spin polarized current [7] and out-of-plane spin-orbit torque [8] needed for field free magnetization switching. The out-of-plane spin Hall conductivity in such 2D quantum materials are estimated to be an order of magnitude higher than the conventional materials.

Finally, 2D magnets are promising owing to their tunable magnetic properties with gating and doping, where the strength of magnetic interactions can be tuned according to the desired applications. However, most of the 2D magnet based spintronic devices are mostly limited to cryogenic temperatures. We reported above room temperature van der Waals magnet-based spinvalve [9,10] and spin-orbit torque memory [11] devices. In the latter case, we could demonstrate field-free magnetization switching utilizing the co-existence of ferromagnetic and antiferromagnetic orders with intrinsic exchange bias in the system giving rise to a canted magnetism. These findings open a new platform for realizing devices using all-2D heterostructure devices.

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Figure: Schematics for realized 2D devices for spin based logic, spin-valve and memory at room temperature. (a) Graphene majority spin logic device with three in-puts and one output nanomagnets on graphene spin circuit. (b) van der Waals magnet Fe₅GeTe₂ based graphene spin valve. (c) van der Waals magnet based spin-orbit torque device.

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Nanopores for reading single proteins

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Abstract

Nanopores are versatile tools for analyzing a wide array of biomolecules at the singlemolecule level. Recent efforts focus on applying nanopores for sequencing of single proteins. We developed a technique based on the principles of nanopore DNA sequencing that can analyze single peptides and discriminate variants with very high accuracy. In our approach, a peptideoligonucleotide conjugate is slowly pulled through a MspA nanopore by a Hel308 helicase motor enzyme. As the enzyme steps along the DNA portion of the molecule, the peptide is slowly ratcheted through the nanopore, and the corresponding ion-current trace depends on the sequence of amino acids within the peptide. We previously applied this method to detect single amino acid substitutions on peptides (1) and post-translational modifications (PTMs) on immunopeptide sequences with cancer-associated phosphorylated variants (2). We reliably discriminated peptide sequences with one or two closely spaced phosphates with 95% accuracy for individual reads of single molecules.

After introducing the concept, we will present our latest efforts where we explore the possibilities of the technology for more in-depth studies of PTMs. Specifically, we will present research on a plant pentapeptide (YIYTQ) that is known to carry two tyrosine PTMs (3). With our system we can accurately distinguish tyrosine sulfation and phosphorylation PTMs (with near-identical mass of 79.957 Da and 79.966 Da respectively). Furthermore, we can precisely identify the location of each PTM with >96% accuracy on single-molecule level.

Next to these efforts on protein sequencing, I may also present our latest data for trapping and studying single proteins with the NEOtrap (4), as well as our work on the transport of nuclear transport receptor proteins through ultrawide origami nanopores that mimic the nuclear pore complex (5).

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Can AI-based structure predicting methods learn the biophysics of proteins?

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Abstract

ESM-2 is a recently developed protein language model (pLM) trained to predict amino acids that have been masked out of protein sequences. It has been discovered that information about the protein's structure emerges in the internal feed-forward layers of the language model [1]. To what extent this model understands the physics of protein folding and function is an open question. Here we explore the correlation between the internal representation of a large dataset of GFP mutants and their experimentally assayed levels of fluorescence [2]. We find that some of the internal layers do have significant predictive power for the fluorescence level.

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ABC transporters are billion year old Maxwell demons

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Abstract

Starting from structural and biochemical data, we show that ABC transporters, possi bly the most widespread family of transmembrane proteins whose role is to shuttle mole cules across membranes, are a billion years old realisation of autonomius Maxwell demo ns, whose function can be interpreted in terms of measurement, feedback and reset preci sely as stated by Landauer and Bennet.



Figure 1. Schematic steps of the functioning of ABC transporters, pointing to similarities (made rigorous in this work) with Maxwell demons

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Spatiotemporal Techniques for Enhanced Optoelectronic Neuromodulation

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Abstract

Electrical neuromodulation encompasses devices and protocols for neural stimulation [1], neural blocking, and neural monitoring, as well as their use in developing smart and personalized electroceuticals. Electrical neuromodulation is typically conducted using implanted wired devices, usually battery powered. The invasive nature of bulky devices, connected to stimulation electrodes by wires, can cause discomfort at best, and inflammation, infections, and tissue damage at worst. Implantable, flexible, physiologically stable and biocompatible sub-mm wireless devices capable of both neurostimulation and neural blocking, as well as of integration with biosensors in feedback loops and IoT environment, would eliminate the patient discomfort and other complications, and would simultaneously enable targeting a wide range of possible therapeutic targets such as branches of peripheral nerves close to the target organs, a goal up to now impractical with the state-of-the-art technology. We propose enhancing the state-of-the-art technology of wireless optoelectronic neurostimulation devices by optimizing for kilohertz frequency operation and utilizing paradigm-shift stimulation protocols, increasing the efficacy of the devices while simultaneously achieving further device miniaturization.

We will demonstrate the performance enhancement gained by the spatio-temporal optimization of the device geometry and the stimulation protocol. Our goal is device verification, both in-silico and in-vivo, in several laboratory models. Finally, our results would pave the way for future applied translational medical research.

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Can AI-based structure predicting methods learn the biophysics of proteins?

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Abstract

ESM-2 is a recently developed protein language model (pLM) trained to predict amino acids that have been masked out of protein sequences. It has been discovered that information about the protein's structure emerges in the internal feed-forward layers of the language model [1]. To what extent this model understands the physics of protein folding and function is an open question. Here we explore the correlation between the internal representation of a large dataset of GFP mutants and their experimentally assayed levels of fluorescence [2]. We find that some of the internal layers do have significant predictive power for the fluorescence level.

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Altermagnetic lifting of Kramers spin degeneracy

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Abstract

Kramers spin degeneracy refers to the fact that in a nonmagnetic and centrosymmetric bulk crystal the states with opposite spin coincide. To be able to make use of the electron spin in applications, this degeneracy has to be lifted. This can be done by either breaking the time-reversal symmetry, or by breaking space inversion symmetry in combination with spin-orbit coupling (SOC). The latter forms the basis of Rashba- or Dresselhaus-type spin splitting, and ultimately also of the spin-polarised surface states of topological materials. Time-reversal symmetry is broken in materials with magnetic order, but this does not necessarily lift the Kramers spin degeneracy of the spin states (anti)parallel to the magnetisation direction. However, in an antiferromagnet (AFM) the two spin sublattices are connected by translation or inversion symmetry and this maps the electronic structures of the two sublattices on top of each other, thereby restoring the degeneracy. Until the recent introduction of altermagnets (AM) [1,2], these were generally considered to be the two main band structure possibilities for commensurate magnetic order. Here we will present experimental results of the third possibility and show that in altermagnetic MnTe the Kramers spin degeneracy is lifted [3].

Both non-relativistic and relativistic spin effects will be explored and it will be shown how both show up in different photoemission techniques with spin or spatial resolution. Given the high potential of applications of altermagnetic semiconductors, we will show how the spin texture can be controlled and what are future directions in the field.



Calculated and measured electronic structure of the altermagnetic semiconductor MnTe.



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Quantum critical phase of FeO spans conditions of Earth's lower mantle

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Abstract

Earth's interior consists primarily of an insulating rocky mantle and a metallic iron-dominant core. Recent work has shown that mountain-scale structures at the core-mantle boundary may be highly enriched in FeO reported to exhibit high conductivity and metallic behavior at extreme pressure-temperature (P-T) conditions. However, the underlying electronic processes in FeO remain poorly understood and controversial. Here we systematically explore [1] the electronic structure of B1-FeO at extreme conditions with large-scale theoretical modeling using state-ofthe-art embedded dynamical mean field theory (eDMFT). Fine sampling of the phase diagram at more than 350 volume-temperature conditions reveals that, instead of sharp metallization, compression of FeO at high temperatures induces a gradual orbitally selective insulator-metal transition. Specifically, at P-T conditions of the lower mantle, FeO exists in an intermediate "quantum critical" state, characteristic of strongly correlated electronic matter. Transport in this regime, distinct from insulating or metallic behavior, is marked by incoherent diffusion of electrons in the conducting t_{2g} orbital and a band gap in the e_g orbital, resulting in moderate electrical conductivity (~ 10⁵ S/m) with modest P -T dependence as observed in experiments. FeO-rich regions in Earth's lowermost mantle could thus influence electromagnetic interactions between the mantle and the core, producing several features observed in Earth's rotation and magnetic field evolution.

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Coupled Nanopores for Single Molecule Detection

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Abstract

Beyond atomically thin 2D nanopores, we conceptualize, simulate, and experimentally demonstrate coupled, guiding, and reusable bilayer nanopore platforms (GURU), enabling advanced ultrafast detection of unmodified molecules. The bottom layer can collimate and decelerate the molecules under detection, and the top 2D pore enables accurate sensing. We varied the number of pores in the bottom layer from one to nine while fixing one 2D pore in the top layer. When the number of pores in the bottom layer is reduced to one, sensing is performed by both layers, and distinct T- and W-shaped signals indicate the precise position of molecules and are sensitive to fragment lengths. This was enabled by microsecond resolution capabilities and precise nanofabrication. Coupled nanopores present configurable systems for improved electromechanical control and prolonged dwell times.



Schematic of a bilayer nanopore platform consisting of one 2D pore on top of one SiN pore. The two pores are at distances comparable to the pore sizes and their electric fields are overlapping and coupled. This is in stark contrast to two far apart, independent pores in series, which have been topics of previous research. In this work specifically, a 2D MoS₂ pore was fabricated on top of the SiN trench and pore.

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Designing Next-generation XNA-based Invader Probes Enabling Sequence-specific Duplex Invasion for Advanced Biomedical Applications

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Abstract

The development of robust oligonucleotide probes that can recognize specific sequences of dsDNA is crucial for various biomedical applications including target detection, gene editing, and DNA data encoding. Invader probes have been developed with the ability to bind DNA through several invasion modes including triplex or duplex invasion.¹ In triplex invasion, the target DNA must be homopurine which limits the number of suitable target sites, making duplex invasion a more versatile and more widely exploited binding mode. Existing strategies for duplex invasion, however, suffer from major limitations including poor probe stability, low invasion efficiency,² and/or dependence on enzymes.³ A more robust strategy involves the use of synthetic nucleic acid mimics, known as xeno nucleic acids (XNAs), which offer superior stability and may resist degradation by enzymes and extreme physicochemical conditions. Among them, peptide nucleic acids (PNAs), characterized by their neutral pseudopeptide backbone, can bind complementary nucleic acids through various binding modes via Watson-Crick and/or Hoogsteen base pairing rules.^{4,5} Thus, they have found applications in PNA-assisted cleavage of DNA and RNA,^{6,7} target identification,^{8,9} and data encoding.¹⁰ To enhance their invasion efficiency, standard PNA probes have been advanced through chemical modifications of their backbone at the α or γ position, or via conjugation of their N or C-terminus with functional peptides.^{5,11} Herein, we present the rational design of advanced PNA-based invader probes that combine synergistic strategies for enhanced, sequence-specific duplex invasion. We demonstrate the design, synthesis, characterization (CD, LC-MS), and validation of the probes and their invasion capacity through electrophoretic mobility shift assays. With their versatility, sequence-specificity, and high efficiency, these next-generation XNA-based invader probes show immense potential to enable a range of biomedical applications relying on sequence-specific recognition of dsDNA.

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Quantum defects in 2D semiconductors

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Abstract

Atomic defects in semiconductors are an attractive building block for solid-state quantum technology. In 2015, defects in two-dimensional (2D) semiconductors such as monolayer WSe₂ were found to exhibit single photon emission, attracting great attention as promising candidates in quantum photonic devices. These 2D semiconductors, characterized by strong excitonic effects, are expected to host a variety of defect-bound excitons that are rich in physics, inheriting the unique properties of the host crystal. However, the structural and physical origin of bound excitons remains elusive, hindering strategic defect engineering. I will first discuss controlled insitu and ex-situ generation of atomic defects in the dilute limit where quantum effects are observed [1, 2]. I will then discuss determination of the many-body nature of bound excitons through electro- and magneto-optical spectroscopy [2,3]. Finally, I will discuss our findings on single atomic defect conductivity and photoconductivity, demonstrating an innovative method for rapid and precise quantification of select impurities in the dilute limit (<10¹⁰ cm⁻²) under ambient condition [4].

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Memory effects in nanofluidic channels: toward brain-inspired ionic computing

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Abstract

The study of memory in nanofluidic channels is a recent and dynamic research topic^{1,2}. Solidstate electronic memristive devices have been the object of intense research for more than a decade resulting in the rise of brain-inspired, or neuromorphic, computing. In comparison, inmemory processing with fluidic nanodevices relying on ions as information carriers is only starting. It provides however a better analogy with biology as the brain relies on billions of ionic nanochannels to perform information processing at energy costs orders of magnitude lower than electronic digital circuits. Thus, developing nanofluidic neuromorphic systems is an effort aiming at reproducing the extraordinary computing performances displayed by brains of living organisms. In this presentation, I will narrate the birth of brain-inspired nanofluidics. I will describe the original nanofluidic memristor, the activated carbon nanochannels³ and its direct evolution, the highly asymmetric channels⁴. In particular, I will discuss how these devices are fabricated and characterized and comment on their performance and potential. I will disclose the physical mechanisms leading to the emergence of ionic memory in these channels. I will then show how these devices can be used for computing applications like Hebbian learning or logic gating at the circuit scale. Finally, I will open the discussion on the advantage of ion-based computing against conventional electronics and the future directions to move the field forward.

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Interface-induced superconductivity and tunable topological electronic structure in Fe(Te,Se)/Bi4Te3 heterostructures

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Abstract

The fabrication of heterostructures with atomically sharp interfaces is a widely used approach for creating and controlling exotic quantum phenomena resulting from the interplay of topology and electronic correlation. For example, superconductivity driven into the topological phase is associated with the formation of Majorana fermions that are of great interest for enabling fault tolerant quantum computation. Here we explore the interface between a Bi-Te topological insulator system and the unconventional superconductor Fe(Te,Se). Previously we demonstrated that the Fe(Te,Se)/Bi₂Te₃ system is a highly tunable platform for realizing topological superconductivity [1]. The new finding is that for low Se fractions the superconducting transition temperature (T_C) of Fe(Te,Se) increases from nominally non-superconducting to as high as 12.5 K when the composition of Bi₂Te₃ layers reveal that a large electron transfer, epitaxial strain, and novel chemical reduction processes are critical factors for the enhancement of superconductivity [2]. This novel route for enhancing T_C in an important epitaxial system provides new insight on the nature of interfacial superconductivity and a platform to identify and utilize new electronic phases.

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Fluorescent nanodiamonds as nanoscale sensors for biological systems

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Abstract

Fluorescent nanodiamonds, harboring optically active defects, serve as both highly stable optical markers [1] and a promising platform for achieving nanoscale sensitivity and resolution in sensing applications [2-5]. The most known diamond color center is a Nitrogen-Vacancy (NV) center, which can be applied for various sensing protocols, including observation of magnetic [2] and electric [3] fields as well as temperature monitoring [4]. Other potentially interesting diamond defects are Silicon-Vacancy (SiV) and Germanium-Vacancy (GeV) centers, which can be used as thermometers [5].

Fluorescent nanodiamonds are fascinating systems for biomedical applications. It is based on the following points: diamond is an inert and nontoxic material [6]; nanodiamond surface can be chemically functionalized for different purposes, including drug delivery [7]; nanodiamonds can be used for theranostics [4].

The biological application of fluorescent nanodiamonds is strongly connected to their surface modification [4, 5, 7]. Furthermore, the sensing capabilities of nanodiamonds are profoundly influenced by their surface characteristics. Here, we are going to discuss the current sensing achievements of fluorescent nanodiamonds for measuring biological systems, as well as explore potential limitations and strategies to surmount them.



Figure 1. The structure of diamond color centers. NV sensing - changes of optically detected magnetic resonance (ODMR) line. SiV and GeV sensing - the temperature-related shift of zero-phonon line (ZPL).

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Skyrmion manipulation using electrical currents and thermal gradients

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Abstract

Magnetic skyrmions show promise for future data storage applications due to their topological protection and easy manipulation. An electric current exerts two forces on the skyrmions: a drag force parallel to the current and a Magnus force perpendicular. When these forces overcome pinning effects, they drive a translation of the skyrmions. Here, I will discuss recent small-angle neutron scattering (SANS) studies, showing how the skyrmion lattice (SkL) may be manipulated by radial electrical and thermal currents.

In the first part, I will discuss results on the SkL in MnSi under the influence of radial electric and thermal currents. Using a (semi)circular sample the electrical current has a 1/r dependence, resulting in a torque on the SkL and leading to rotation to a new static orientation relative to the MnSi crystalline axis. Interestingly, the rotation shows a nonmonotonic current dependence, changing direction at high currents. We understand the switching to be due to a competition between the electrical current and the accompanying thermal current due to Joule heating.

Motivated by the results discussed above, we studied the SkL in insulating Cu_2OSeO_3 under a thermal gradient. Again, a radial configuration was used, with a heater connected to the center of a disc-shaped sample. An array of temperature sensors affixed to the sample ensured accurate measurement and determination of the temperature profile. By changing the sample temperature, it is possible to vary the torque, due to the thermal gradient, relative to the crystalline anisotropy that selects a preferred SkL. At higher temperature, closer to the paramagnetic transition, a static reorientation of the SkL is observed similar to the situation for MnSi described above. However, as the temperature is lowered and one approaches the conical phase, a continuously rotating SkL is obtained. I will show how it is possible to image the rotating SkL using time resolved SANS measurements.

Proximity effects in van der Waals materials

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Abstract

Graphene has weak spin-orbit coupling and no magnetic order. But when placed in contact with a strong spin-orbit coupling material, such as a TMDC, or a ferromagnet, such as Cr2Ge2Te6, Dirac electrons acquire strong spin-orbit or exchange coupling, respectively. Such proximity effects render graphene suitable for spintronic applications that require spin manipulation [1]. Graphene with strong proximity spin interactions can host novel topological states [2], or form ex-so-tronic devices [3] which offer spin swap functionalities: switching spin-orbit and exchange coupling on demand by gate. I will review the recent developments in the proximity phenomena in graphene, and present new theoretical results on the control of the proximity spin-orbit and exchange coupling by twisting the van der Waals layers [4, 5]. Finally, I will also discuss the emergence of new correlated phases in graphene [6] due to the presence of proximity spin-orbit and exchange couplings, and the routes towards radial Rashba interactions [7]. Support from DFG SPP1244, SFB 1277, FLAGERA 2DSOTECH, and Graphene Flagship 2DSPIN-TECH is acknowledged.

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Imaging and Sensing with glass Nanopores

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Abstract

Scanning ion conductance microscopy (SICM) has been around for decades [1], yet it has not received as much attention as other forms of scanning probe microscopy. Recently, this true non-contact technique has kindled renewed interest among biophysicists and biologists because it is ideally suited for label-free imaging of fragile cell surfaces where it achieves exquisite resolution down to the nanometer regime without distorting the cell membrane. SICM uses a glass nanopipette as a scanning probe and measures the current through the glass nanopore as a proximity detection of the sample surface [2]. The challenge to harness this technique for time resolved 3D nanocharacterization of living cells lies in the relatively slow imaging speed of SICM. In this presentation I will show how we apply what we have learned from high-speed AFM to the field of SICM. By reengineering the SICM microscope from the ground up, we were able to reduce the image acquisition time for SICM images from tens of minutes down to 0.5s while extending the imaging duration to days [3].

SICM, however, is much more versatile than just an imaging tool. I will also discuss our recent results using SICM as a single molecule characterization tool. We term this method scanning ion conductance spectroscopy (SICS) [4]. Using capillaries with exceptionally small nanopores, we can detect and manipulate single molecules in a repeatable and high throughout manner. Compared to other nanopore sensing techniques SICS has inherent temporal and spatial control of the DNA translocation through the nanopore. This greatly increases the SNR and enables detection of even single base gaps in a dsDNA strand. The ability to read the same molecule multiple times makes this technique well suited for biophysics and diagnostic applications.



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Reading amino acids with ultrathin nanopores

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Abstract

Nanopore based protein sequencing is attracting rapidly growing research interest due to its single molecule, portable and electric readout features. However, protein sequencing using nanopores still faces challenges related to the required spatial and temporal resolution to discriminate single amino acids in a peptide chain. Our group develops ultra-confined nanopore structures, nanofluidic approaches and biophysical understandings that promote the measurement resolution. We recently optimized the precise and controllable fabrication of ultrathin MoS₂ nanopores and demonstrated the direct experimental identification of single amino acids. With ultra-confined regions of sensitivity, MoS₂ nanopores can read the tiny chemical group difference of single amino acids, and 16 out of 20 types of natural amino acids can be identified in a same nanopore. The direct discrimination of isomers and post-translational modifications of individual amino acids was further allowed with such a nanopore. We believe that nanopores with subnanometer confined region may provide opportunities for ultrasensitive molecular analytics such as protein sequencing.

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Imaging real-time single-molecule dynamics in genome regulation

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Abstract

The dynamic organization of the eukaryotic genome into chromatin is integral to gene regulation. Chromatin controls genome access for DNA binding factors, and is regulated by multiple dynamic processes, including nucleosome remodeling and the installment and removal of post-translational modifications (PTMs).

We develop single-molecule colocalization imaging [1] and single-molecule FRET approaches [2] to directly observe the complex dynamics underlying chromatin regulation in gene activation and repression. Genes are controlled by transcription factors (TFs), which need to invade chromatin structure from the nucleosome to the larger chromatin fiber level. A subset of these factors, pioneer TFs, have evolved strategies that allow them to efficiently search and bind to compact chromatin. Our studies, combining in vitro and in-cell single-molecule experiments show that intrinsically disordered regions flanking the DNA binding sites of pioneer TFs are key for an efficient search and pioneer activity, whereas bound TFs control the activity of chromatin remodelers to clear promoter regions of nucleosomes. Conversely, the deposition of histone PTMs, including H2A ubiquitylation, is critical for gene repression. Using multi-color single-molecule imaging, we observe how the responsible ubiquitin ligase, PRC1, searches and binds and modifies chromatin in a concerted reaction, resulting in structural changes altering gene expression [3]. Our method allows us to reveal individual reaction steps in real-time, enables us to determine the enzymatic mechanisms at play and allows us to identify protein-protein interactions that are key for allosteric control of PRC1 and reveal chromatin states that are specifically targeted.

Overall, our results show how chromatin modifications control overall chromatin structure and thus gene expression programs, and how pioneer TFs can overcome such a barrier, providing mechanistic insights into chromatin regulatory processes.

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Substrates for the research of micro-topographic and galvanotropic cues for axonal guidance

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Abstract

During brain development axons grow towards their goal with a high degree of accuracy. Chemical, topographical and galvanotropic cues are responsible for their guidance. Research of external cues for axonal guidance is vital because of possible clinical applications, such as accelerating nerve regeneration after traumatic injuries, as well as for further scientific research (e.g. characterization of living neural networks). We designed and produced substrates with different topographical and galvanotropic elements which can be used for further investigation of axonal guidance. Microstructuring of the surface is done by using nanosecond and femtosecond laser ablation. Materials used for the substrates are borosilicate glass (dielectric) and silicon (semiconductor) on which the effects of different duration and energy of laser pulses are seen. Characterization is done by using an optical profilometer, a contact profilometer and a scanning electron microscope. The dependence of ablated volume, diameter and depth of ablation craters for different pulse energies is measured. The ablation threshold fluence is determined by the D^2 method. Organic electrolytic photocapacitors (OEPCs) were used for galvanotropic cues. OEPCs are optoelectronic stimulators based on a p-n bilayer of organic semiconductors which are used for capacitive neurostimulation. It has been demonstrated that they generate sufficient electrical charge to modulate neural tissue in vivo¹. Using a nanosecond and a continuous laser, a designed pattern of a p-n bilayer is removed from the surface of the photocapacitor, thus making an inverse photocapacitor. Characterization of said inverse photocapacitors is done by measuring the transient electric potential.

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Kirgami electronics for organoids: towards interfacing complex tissues

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Abstract

Brain organoids are enabling the non-invasive study of human neural development and capturing phenotypes of disease. Cardiac organoids pave the way for regenerative medicine. Accessing the electrical activity of these electrogenic organoids is central to understanding the development and biological faithfulness of these novel tissue platforms. Mesh electrode arrays are low footprint devices that are flexible and conformable. Owing to these features, organoids can integrate the device during their development in-vitro which results in electrodes distributed all throughout and allow long-term recording of electrical activity. Using lithography, we designed micron-thin polymer structures into a mesh which unfolds into a basket in aqueous solution, accommodating organoids in its center point. We have designed devices that are flexible by exploring rotational degrees of freedom of the design inspired by the Kirigami paper cutting art.

Using this design, we can culture and record from organoids on these meshes for over 180 days.



Figure 1: Kirigami Electrode Array. a) Kirigami-inspired electrode-array that unfolds under gravity and the weight of the organoid (green). b) The shape of the organoid (round) is preserved and not disturbed by the inclusion of the device.

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Topological superconductivity in twisted doublelayer high-Tc cuprates: Theory, experimental signatures and applications

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Abstract

Structures composed of two monolayer-thin *d*-wave superconductors with a twist angle close to 45° are predicted to form a robust, fully gapped topological superconducting phase with spontaneously broken time-reversal symmetry and protected chiral edge modes. In this talk I will briefly review the theory behind the topological phase and discuss recent experimental efforts to fabricate and probe twisted flakes of high- T_c cuprate Bi₂Sr₂CaCu₂O_{8+ δ}. Signatures of *d*-wave symmetry and of spontaneous T-breaking are indeed visible in the device Josephson current response, as detected through a pronounced superconducting diode effect observed in samples near 45° twist but absent in untwisted samples. Time permitting, a potential application of this physics to an improved transmon qubit will also be discussed.

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Transfer, coupling and bonding of ions in CNT porins

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Abstract

Narrow sub-nm carbon nanotubes (CNT) porins are unique mimics of water channels in biological membranes. Their selectivity towards ions has been demonstrated by stop-flow measurements of ion diffusion in vesicles and single-pore I-V measurements. Many insights that can help interpret such data were also gained by continuum electrostatic models as well as MD and *ab initio* simulations, however, most computations do not include ion specificity or do not capture it with sufficient accuracy. Another challenging aspect, critical for interpreting experiments, especially in ion diffusion measurements, is ion coupling, which affects the physical meaning of parameters derived from experiments. To address these challenges, we employ ab initio simulations of high theory-level to compute free energies for transfer of individual ions and ion pairs from solution to the interior of short CNTs surrounded with a dielectric continuum.

We find that, in agreement with previous simulations, highly favorable and chemical bonding-like interactions of cations with CNT, allow their transfer of cations in the "electroneutrality breakdown" (EB) mode, i.e., as a single ion at a time, without local coupling to anions. On the other hand, anion transfer in EB mode involves prohibitively large energy and must be locally coupled to cation transfer, i.e., anions may only be present within CNT simultaneously with a cation. We differentiate two limiting regimes of such simultaneous transfer, strong coupling (SC) when the two ions form a pair and weak coupling (WC) when both ions retain translational freedom. The computation of associated transfer energies is greatly facilitated by the remarkable finding that CNT behaves as highly polarizable metal-like volume thus polarization energy vanishes both in SC and WC, promoting coupled ion transfer. Based on this finding, we compute and systematically compare the transfer costs in different coupling regimes, which helps identify the most favorable mode for each ion. WC mode appears somewhat more favorable for chloride, while larger halides and OH⁻ favor SC, i.e., transfer mainly as ion pairs. The results suggest that experimentally observed pseudo-linear anion diffusion kinetics most likely reflect ion-pair (SC) permeability, not uniquely defined by the anion and dependent on the counter-ion present in the buffer as well. Implications of these results for CNT conductivity and effects of pH are also discussed.

Giant X-ray circular dichroism in a time-reversal invariant antiferromagnet

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Abstract

Structurally chiral molecules and crystals including various bio-molecules exhibit strong natural circular dichroism (NCD) in the visible-to-ultraviolet region, but NCD in the x-ray region (XNCD) is orders of magnitude weaker than x-ray magnetic circular dichroism (XMCD) that is observed in ferromagnetic and ferrimagnetic materials, where time-reversal symmetry is broken. Collinear antiferromagnetic materials with time-reversal symmetry do not show any XMCD because of the fully compensated spin moments except for "altermagnetic" materials, where time-reversal symmetry is broken.

We report on the observation of a new type of strong XNCD at the Ni L_3 edge of the structurally chiral, collinear antiferromagnet Ni₃TeO₆ [1], although the material has time-reversal symmetry in the ground state and hence should normally exhibit only faint XNCD. To explain the strong XNCD, we propose a mechanism involving the time-reversal-symmetry breaking caused by the x rays incident on the chiral crystal.

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Unraveling the anomalous dielectric properties of interfacial and nanoconfined water

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Abstract

In this contribution, I will talk about our work in which we experimentally investigate the dielectric polarization properties of near-surface and confined water. These properties have long been subject of research because they are critical to a variety of phenomena, including surface forces, ion/molecular solvation and transport, and chemical reactions. However, they have remained essentially unknown for great difficulties in measuring them. After briefly introducing our experimental setups that are based on advanced scanning probe methods [1-3], I will discuss our recent results in which we directly measured the dielectric properties of few water layers confined inside nanochannels made of van der Waals crystals [4,5]. Our experiments revealed the presence of an interfacial water layer with dielectric properties that greatly differ from those of bulk water. Our results open up new possibilities for understanding many natural processes, providing important feedback for theories describing water-mediated interactions.

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Electric Cell-Substrate Impedance Sensing (ECIS) system for cell dynamics monitoring: from monolayer to single cell

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Abstract

Deep into the intricate mechanisms that direct cell migration, particularly those acting on focal adhesion and intracellular force generation ¹ is critical to enhance the comprehension of certain disease developmental processes, such as tumor migration, neuron disorder; therefore, to pave the way for potential therapeutic interventions targeting cell migration based fundamental diseases disorders.

Electrical cell-substrate impedance sensing (ECIS) stands as a robust in vitro monitoring technique for cultured cells, with a primary focus on cell-chip adhesion and migration. ² In the conventional ECIS systems, there is a significant difference in surface areas between the working electrode (WE) and the counter electrode (CE), with the latter being several hundred times larger (Figure 1). By applying an alternating current or voltage between the WE and CE, the cell growth dynamics could be monitored by tracking the impedance of the cell-covered electrode, the cell-chip impedance measurement is therefore dominated by the electrode-electrolyte interaction that happens at WE interface.

However, in the case of small sized cells, *e.g.* primary neurons and immune cells ³, the utilization of WE and CE configurations for neuron-electrode impedance measurement under ECIS system features a great challenge. As the impedance contributions from the metalelectrolyte interface of the working electrode are overshadowed by the large impedance of the noble metal electrodes, which strongly decreases the accuracy in monitoring the neuron (small-size cells) behaviors. Here, organic field effect transistor and electrochemical transistors (OFET and OECT) ⁴ are introduced for such impedance measuring with the ability in amplifying the cell potentials change. ⁵

In this work, an impedance based technique is developed for real-time cell dynamics monitoring, novel concepts in electronic designs, *e.g.* using transistor transfer function, are introduced to measure different cell types with various parameters.

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Figure 1: Illustration of ECIS measurement for different cell types. (a) ECIS for wound healing assay measurement, epithelial cells forming confluent layers on typical ECIS device with electrode diameter of 250 μm (https://www.biophysics.com/; 16.02.2024); (b) A cytotoxic T cell extracted from human blood adheres on top of a transistor gate with a dimension of only 12x5 μm². The size of a transistor gate is comparable to a single cell resolution. ³

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Optical control of nanodevices using metal-to insulator-transition and nanostructures

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Abstract

We present here a study of local heating for the control of the physical properties of nanomaterials and the performance of nanodevices. Almost all the physical properties of materials (electrical, magnetic, optic or mechanical) are temperature dependent. Therefore, inducing local heating in nanometric regions allow to modify locally different properties as resistivity, magnetization, refraction index or induce mechanical stress via thermal dilatation. While the dependence of physical properties with temperature is normally monotonous and soft, some materials exhibit phase transitions where physical properties changes significantly in a small temperature interval. At these phase transitions, strong variations of the physical properties can be induced with a small change of temperature. In addition, as many external stimuli can induce local heating, this method provides a path to couple via local temperature different properties (e.g change magnetization upon illumination, change of transmittance with magnetic fields, etc) in materials that do not show this coupling naturally.

Up to now, local heating has been used mostly to modify the physical properties of individual nanostructures. Here, we explore the use local heating with ensembles of nanostructures to create patterns of heated regions giving rise to regions with modified physical properties that act as nanodevices. In this way, it would be possible to switch on / off via local heating electrical circuits, magnets or waveguides. Using different types of nanostructures that can be selected locally, we will address the activation of different nanodevices at the same region of space as desired. We face here the fabrication of these devices, methods for measurement of the local temperature, optimization of the control of the physical properties and performance of the devices.

Musical Synchronization and its Role for the Swing in Jazz

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Abstract

Synchronization is a central topic in nonlinear dynamics with many applications across the sciences, from fireflies to active particles. But how do musicians synchronize, when they interact in a perfomance? It is a widespread opinion that they should perfectly synchronize their timing - can this be supported by experiments and data analysis? This opinion was challenged in particular for the swing feel, a salient feature of most jazz styles, which was considered arcane and has long eluded scientific clarification. According to an old conjecture it was rather vaguely attributed to some kind of *desynchronization* between participating musicians. Using data analysis of more than 450 renowned jazz solos and based on various experimental approaches, we clarify this conjecture and determine which synchronization properties and phase shifts between instruments are relevant for the swing feel.

Multimodal Graphene-based Microelectrode Arrays for In-Vivo and In-Vitro Applications

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Abstract

Multimodal platforms combining electrical neural recording and stimulation, optogenetics, optical imaging, and magnetic resonance (MRI) imaging are emerging as promising tools to enhance the depth of characterization in neuroscientific research. This talk will discuss electrically conductive, optically transparent, and MRI-compatible graphene-based in vivo and in vitro electrode arrays to optimally combine all modalities. The electrode arrays are microfabricated on wafers using a unique transfer-free process. Using this process, graphene electrodes on transparent rigid substrates or flexible polymers can be realised. The resulting multlayer, molybdenum-grown, graphene exhibits the highest charge storage capacity (CSC) reported to date among all previously fabricated CVD graphene electrodes. The flexible implantable arrays do not reveal any photo-induced artifacts during optogenetic stimulation nor image artifacts in a 3T MRI scanner. These results demonstrate that multilayer graphene electrodes are excellent candidates for the next generation of neural interfaces and can substitute the standard conventional metal electrodes.

Disorder in Andreev reflection of a quantum Hall edge

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Abstract

We develop a theory of charge transport along the quantum Hall edge proximitized by a "dirty" superconductor. Disorder randomizes the Andreev reflection rendering the conductance of a proximitized segment a stochastic quantity. We investigate the statistical distribution of the conductance in two types of systems: a single v=2 proximitized edge, and two counterpropagating, proximity-coupled v=1 edges. In the latter case, the system is naturally tuned to the critical point between trivial and topological phases by the competition between tunneling processes with or without particle-hole conversion. We investigate the effects of electron density, magnetic field, and temperature on the conductance distribution function.

Tailoring the magnetism of van der Waals materials through molecular intercalation

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Abstract

Intercalation is the insertion of guest species in the van der Waals gap of a host layered material. This process leads to a profound modification of layered material physical properties, due to a significant change in charge carrier density and interlayer distance. The choice of organic molecules as guest species offers multiple tailoring options due to their different size, electronic and magnetic properties [1, 2]. Here, we show that organic-ion intercalation dramatically changes the magnetic properties of layered antiferromagnets NiPS₃, MnPS₃ and CrSBr. While NiPS₃ and MnPS₃ exhibit intra-layer antiferromagnetic response. Specifically, NiPS₃ intercalates show doping-induced magnetization in the order of $10^{-2} \mu_{\text{B}}/\text{atom}$ (Fig. 1) [3], while MnPS₃ intercalates display a saturation magnetization reaching up almost 1 $\mu_{\text{B}}/\text{atom}$. In CrSBr, characterized by intralayer ferromagnetic order and interlayer ordering from antiferromagnetic to ferromagnetic. Our results establish organic-ion intercalation as an effective tool to tune the magnetism of layered materials.



Figure 1. a) NiPS₃ was intercalated with tetrabutylammonium ions (TBA), which were subsequently exchanged with cobaltocenium ions (Co(Cp)₂). b) Magnetic hysteresis recorded for NiPS₃, TBA-NiPS₃ and Co(Cp)₂-NiPS₃ (black, red and blue curves, respectively).

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Low-dimensional materials: it's okay not to be perfect

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Abstract

The story of two-dimensional (2D) materials derived from van-der-Waals (vdW) layered crystal is one of excitement and triumph. 2D vdW materials have received widespread attention due to the plethora of unique properties that can be fine-tuned through control of thickness, twist, interface, or defects. However, the production of 2D materials from a limited library of vdW solids inherently restricts the range of accessible 2D vdW materials and properties based on the finite list of the starting vdW materials. Furthermore, the projected applications of 2D materials often require high structural quality. In this presentation, we will discuss various pathways to expand the portfolio of 2D materials to non-vdW materials and explore applications in which structural disorder is not a hindrance but can provide additional advantages.

Recent reports have suggested that 2D nanosheets could be produced from isotropic, nonlayered, non-van-der-Waals materials. This behavior is very surprising because similar surface energies of the crystal planes in isotropic materials are expected to form three-dimensional (3D) nanoparticles instead of nanosheets. Illuminating the exfoliation mechanism in non-vdW materials would lead to a rational design of an entirely new class of 2D materials with unique properties and applications. By combining synthesis, atomically resolved imaging, and theoretical calculations, we demonstrated that planar defects drive the nanosheet exfoliation in strongly bonded isotropic and non-layered materials. We used boron as a model system and demonstrated that defect engineering provides a clear path for creating low-dimensional boron sheets and other covalently bonded materials by replacing random synthesis attempts with engineerable pathways.

The second example will focus on wafer-scale growth of crystalline, ultrathin (<1 nm), and conformal vdW films using a thermal atomic layer deposition at back-end-of-line (BEOL)-compatible temperature (350 °C). Although our low-temperature process results in polycrystalline films, we demonstrate that our vdW films lead to a significant reduction in Cu resistivity by six orders of magnitude for Cu interconnects that are less than 10 nm thick. These thicknesses are not only technologically relevant but also enter the regime where fundamental physical properties start to break down and limit the material's performance. To date, the commercial use of 2D materials has largely remained unachieved; however, our industry partner is actively working on a commercial product solution based on our 2D films, offering a pathway to integrate 2D materials into commercial applications.

Ohmic conductance of nanofluidic systems: paradigm and beyond

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Abstract

Two decades ago, the Ohmic conductance paradigm of nanofluidic systems was established wherein it was observed that the conductance shifted from a linear concentration dependence on the concentration to one that is concentration dependent (red line in Figure 1). This change occurs as the effects of the surface charge density become more dominant and the system becomes more selective. However, as experimental setups become more elaborate, it appears that this paradigm is incapable of accurately describing observations. In particular, various works have shown that surface charge regulation [1,2], slip lengths [3], and the microchannels [4] can drastically vary the low-concentration slope. Further, the current paradigm is also incapable of predicting the conductance for a system subjected to a concentration gradient.

In this talk, I will survey my lab's efforts [4–6] to show that the current paradigm does not necessarily need to be abandoned and how, through various modifications, the paradigm can be correctly and consistently updated. I will present some of these newer models and the key insights they provide. I will also discuss our lab's future goal of merging all the models into a single universal model.



Figure 1. A nanofluidic system comprised of two microchannels connected by a single nanochannel. The entire system is subjected to a potential drop and concentration gradient. The classical paradigm is given by the red line. A new paradigm is given by the blue line that can be shifted and have a different slope.

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Electrically Pumped GeSn/SiGeSn Multiple Quantum Well Laser

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Abstract

Si-based photonic integrated circuits (PICs) in which optically active components are monolithically integrated on chip are transforming the next generation of information and communication technology infrastructure [1]. In the quest for a fundamental direct bandgap, group-IV semiconductor alloys have been intensely investigated to obtain an electrically pumped, continuous-wave Si-based laser. Along this path, it has been demonstrated that the electronic band structure of the newly developed GeSn/SiGeSn hetero-structures can be tuned, via stoichiometry and strain engineering, into a direct bandgap quantum structure providing optical gain for lasing [2]. In this paper, we present a electrically-pumped laser emitting at a near infrared wavelength of 2.35 µm with a low threshold current of 4 mA (5 kA/cm²) at low temperatures. It is based on a 6 periods SiGeSn/GeSn multiple quantum-well structure deposited on a Si substrate with a relaxed Ge buffer layer. The small footprint micro-disk cavity laser are fabricated by defining a circular Mesa structure. The rim of the disc was underetched by 900 nm by removing the Ge buffer in this area. The remaining Ge pedestal is used as p-contact area as well as heat sink for the laser (Fig 1 a,b). In this simple construction the actual lattice temperature in the active region is about 60K higher than that of the thermal bath T_b, due to the poor heat conductivity of SiGeSn. However, the laser operates in continuous-wave (CW) regime up to T_b=40K, but can also efficiently work in a direct modulation regime down to ns pulses at $T_b=77K$.

A typical high resolution lasing spectrum with a FWHM of $50\mu eV$ is shown in Fig. 1c at T_b=5K and a pump power of 12 kA/cm². The demonstration of a CW, electrically pumped, all-group-IV laser is a major breakthrough towards achieving a complete truly-silicon photonics technology platform. It opens up applications in the rapidly developing mid-infra-red imaging and sensing.

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Fig. 1 a) Elemental map of the SiGeSn/GeSn multiple quantum well structure and associated TEM cross sectionb) Schematic view of the fabricated devcie c) High resolution spectrum showing FWHM of 60 µeV, spectrometer bandwidth 25µeV

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Measuring and Manipulating Spin and Magnetization Dynamics in Two-Dimensional Materials

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Abstract

Van der Waals (vdW) materials are ideal systems for the study of spins and magnetism in low dimensions since they maintain their excellent optical, magnetic and electronic properties down to the atomically-thin limit. Because of their low dimensionality, these materials possess another exciting property, they are extremely sensitive to external stimuli, such as light and electric fields.

In this talk, I will show how we can use ultrashort (fs) laser pulses to detect and control spins and magnetization in vdW systems. After a brief introduction to magneto-optics and ultrafast magnetization dynamics, I will present our recent results on the 2D semiconductor MoSe2[1] where we use ultrashort laser pulses to generate a spin accumulation and study its time dynamics which is controlled by an out-of-plane magnetic field.

I will also show examples on how the magnetization of vdW magnets can be similarly manipulated using ultrashort laser pulses, and how their magnetization dynamics can be efficiently controlled by both magnetic and electric fields. Particularly, I will show how we can control the spin lifetime in the metallic vdW magnet Fe_3GeTe_2 by rotating its magnetization[2], and how electric fields can be used to tune the magnetization dynamics in the semiconducting vdW magnet $Cr_2Ge_2Te_6$ [3].

Our studies illustrate the potential of vdW materials for combining optics, spintronics and magnetism, making them appealing for new opto-spintronic and opto-magnetic device architectures for future integrated photonic systems.

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Nanopore single-molecule experimentation with enzymes

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Abstract

My group has been at the nexus of developing nanopore sequencing of DNA¹ and establishing nanopores as a new tool for single-molecule biophysics. Much of our work is based on the engineered protein pore MspA² as well as detailed understanding of the nanoscopic physics picture. Here, I will show how we use nanopores as an ultra-sensitive single-molecule³ tool with which we can observe enzyme mechanics in real-time as these molecular machines move along DNA or RNA. We easily achieve ten times better position as well as time resolution than optical tweezers, while simultaneously measuring the exact nucleotide sequence within the enzyme. I will show hereto unseen detail in the motion of helicases, DNA and RNA polymerases, reverse transcriptases, *etc.* Besides establishing decisive kinetic enzyme models our method reveals many surprising properties of these enzymes⁴. Using our nanopore experiments we can explore how drugs interfere with enzyme function⁵ or look for entirely new drugs.

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Dipole orientation reveals single-molecule interactions at liquid and hexagonal boron nitride interface

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Abstract

Single-molecule localization microscopy (SMLM) famous for breaking the diffraction limit and extending the study of molecular optics from bulk measurements to the single-molecule level. However, in situ observation of the molecular interactions and dynamics involved in chemical reactions is still a great challenge. Here we utilize the single-molecule activation of pristine hexagonal boron nitride in organic alkane solvents as a platform for guiding the structure identification and dynamics tracking by measuring the dipole orientation of the emitters with the help of the SMLM technique. We chose acetonitrile as in situ probes due to their linear and rigid structure and its highest purity (>99.9%) from a plethora of commercially solvent. By exploiting the property that molecules' morphology and activity in the excited state will be affected by the local environment and thus cause a deflection of the emission dipole orientation, we have observed the molecular interaction and photophysical dynamics between organic molecules and two-dimensional materials. This bridges the gap where researchers need to make trade-offs between molecular structures measurement and the study of high-throughput phenomena simultaneously. This also contributes to the understanding of chemical reaction processes at the molecular level, advances in the field of nanofluids and quantum sensing via native defects.

Developments in translational hyaluronan analysis using solid-state nanopores

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Abstract

The carbohydrate hyaluronan (also known as hyaluronic acid or HA) is an important biological macromolecule that is found ubiquitously in mammalian tissues and biofluids. With its diverse physiological activities ranging from tissue hydration to the regulation of innate immunity, HA is a major factor in human health and disease. Both the abundance and size distribution of HA polymers can have important impacts on its behaviors *in vivo*, but current technologies have significant weaknesses in quantitation, resolution, and/or sensitivity that have limited our ability to study its roles in detail. Our lab has employed solid-state nanopore analysis¹ as a tool to address this gap. Here, I will review our approach, including experimental considerations² and supporting methods, before discussing applications that will include the determination of urinary HA size distribution as a biomarker of disease progression in urinary tract cancer and the analysis of 'inflammation-marked' HA³ (HA covalently-modified with heavy chains from the inter- α inhibitor protein) in mammalian synovitis.

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Detailed analysis of the covalency of the chemical bond

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Abstract

We provide a detailed analysis of some aspects related to the earlier talk on the chemical bonding [1]. Our method of approach is based on the exact diagonalization combined with the *ab intio* calculations introduced earlier (EDABI) [2], as applied to the two-atomic molecules. In this method we include the electron-electron interactions and solve exactly the extended Heitler-London model. Namely, we combine the first and second quantization descriptions in the sense that the two-electron states are obtained in the latter language, whereas the single-particle wave function determination is carried out in the first-quantization scheme. Here the calculation steps are reversed as compared to the standard analysis of many-particle system. The main results are summarized in Fig. 1, where the electron density profiles for two interatomic distances (R) are depicted on the left and various dynamical energy contributions to the total (bonding) energy are shown on the right. The physical implications of the evolution with the increasing R are related to the other contribution [1].

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Figure 1. Two-particle density (left) and the dynamical contribution to the total (bonding) energy (right).

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Interface Nanopores - Dynamic Nanopore Sensors for Single-Molecule Analysis

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Abstract

Over the past two decades, nanopore sensing has revolutionized single-biomolecule sensing, with applications ranging from DNA sequencing to protein analysis. Recent publications showcased the possibility to differentiate between 20 different amino-acids using state-of-the-art protein nanopores [1-3]. However, existing biological and solid-state nanopores face challenges such as limited flexibility and stability. In this work, we present interface nanopores where sizeadjustable nanopores are formed at the interface of two substrates: one soft and one rigid. By modulating the force applied at the interface, the dimensions of the nanopore can be dynamically modified with single-nanometer precision, allowing for size-specific sensing of any molecule of interest. The two-substrate design and the microfluidic implementation further facilitate functionalization of the nanopore with bioreceptors, e.g. aptamers. This enables specific bioreceptor-target interactions, which results in slower translocation speeds of the target molecules [4]. Hence, this design enhances the spatial and temporal resolution compared to stateof-the-art nanopore sensors. We support our experimental results with COMSOL simulations of various channel geometries. This nanopore sensor promises to advance single-molecule detection and analysis, thanks to its flexibility in size and specificity achieved through mechanical and chemical modulation of the pore.

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Slope of H_{c2} close to T_c versus the size of the Cooper pairs: The role of disorder in Dynes superconductors

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Abstract

The size of the Cooper pair ξ_{pair} is one of the basic characteristics of a superconductor, but it is not possible to measure it directly. It has been suggested that ξ_{pair} can be determined from the value ξ_{slope} extracted from the measurement of the slope of H_{c2} close to T_c. Taking into account both pair-conserving and pair-breaking scattering on impurities within the recently developed theory of Dynes superconductors, we perform an explicit calculation of ξ_{pair} and ξ_{slope} . We show that the two quantities agree only in clean superconductors. In particular, when the pair-breaking disorder approaches the quantum critical point, ξ_{pair} stays finite, whereas ξ_{slope} diverges.

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Design and construction of a Nitrogen-Vacancy mediated Optical Detection Magnetic Resonance (NV-ODMR) Spectrometer, a high density quantum sensor platform

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Abstract

Fluorescence detection of an individual Nitrogen-Vacancy center (NV-) in diamond enables to identify and locate other spin holding atoms within a \sim 30 nanometer radius sphere using Magnetic Double Resonance experiments. A plethora of applications based on ingenious experiments have been envisioned using individual NV centers as qubit-based quantum sensors. However, to gain practical information, these single molecule experiments must be repeated millions of times — while scanning over a surface or collecting statistics of reversible chemical processes through long time observation — making the measurement time unpractically long. An alternative approach is to build a measurement platform where 106 – 108 quantum experiments are run parallel on less than a cm² diamond surface, using subsurface NV centers, the longest room temperature coherence time qubits.

The long-term aim is to create a bio-analytical instruments capable of quantitative mapping of the human proteome [1] in personal (home) setting — a potential game changer of diagnostics and healthcare. First, I will describe the concept of such an instrument and proceed to define the technical parameter space for its realization. Then identifying the challenges I describe the development direction chosen, a combination of an L band pulsed EPR spectrometer with a fluorescence imaging system build around a 100nm thin diamond chip placed in a micro fluidic cell. I will describe the current status of the instrument construction and address the remaining design challenges.

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Lessons from the Hubbard model: from high-Tc superconductivity to altermagnetism

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Abstract

The Hubbard model is the paradigmatic model of correlated electrons on a lattice. Its realizations on various lattice geometries have been studied intensely for their relevance to correlated materials, ranging from the high-Tc cuprate superconductors to the newly discovered class of magnetic systems known as altermagnets. Although the Hubbard model has no analytic solution, there has been significant progress over the past several years in understanding its essential physics owing to advances in numerical simulation techniques. In this talk I will highlight some of the lessons we have learned recently from Hubbard model numerics, focusing on exact, finite-temperature quantum Monte Carlo simulations. I will showcase our results concerning spin and charge density waves in the 2d square lattice Hubbard model and discuss their connections to mysteries in the cuprate phase diagram. I will also discuss preliminary data from quantum Monte Carlo simulations of altermagnetic Hubbard models, illustrating the utility of model as a platform for understanding the emergent properties of novel phases of matter.

Understanding biological neurons: Insights from small-scale neuronal cultures

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Abstract

One of the biggest challenges in neuroscience is understanding how the brain can learn, and store information. Despite many valuable efforts undertaken by the field, the precise mechanisms governing learning and memory remain mostly elusive. In this work, we do not attempt to unveil the enigma by looking at the brain as a whole; a concept followed in top-down neuroscience. Instead, we apply bottom-up neuroscience paradigms, where we investigate the dynamics of only a few neurons in-vitro.

In-vitro culture can be created by dissociating brain tissue. The resulting cultures can contain anywhere from thousands to hundreds of thousands of neurons [1,2]. Consequently, the cultures are still relatively complex. To further simplify the neuronal cultures, we impose physical constraints, that limit the way neurons can connect with each other [3,4]. With such constraints, we can achieve cultures that have fewer than 100 neurons. Their electrical activity can be recorded using micro-electrode arrays (MEAs).

In this work we investigate the network activity of small dissociated neuronal cultures continuously over multiple weeks of their development. We also present tools we developed that make such a task possible. We further stimulate the cultures electrically and show the effects of stimulation amplitude and timing on the spiking activity. We found that our cultures have unique, yet reliable responses to distinct types of stimuli [5].

Finally, we present ongoing work, where we observed promising plasticity effects in our cultures. Plasticity research in dissociated cultures is famously unreliable [6]. We uncover plasticity paradigms that can be reproducibly found in many cultures.

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Inorganic/organic hybrid materials in transistor arrays for biomedical applications

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Abstract

For the *in vitro* monitoring of cells and tissue and for organ-on-a-chip applications, commercial solutions exist integrating many devices (>25k) in one chip. These devices are typically fabricated in classical complementary metal-oxide semiconductor (CMOS) processes. They demonstrate low-noise recording capabilities and ultra-high integration of with sensor-to-sensor pitches of only 20 micrometers and less. In addition, most of the systems offer spatially resolved electrical stimulation. Most of the time, however, post-processes are needed to enable a long-term operation in liquid environment and integration of reference electrodes to stabilize the liquid potential. For all such silicon-based devices, the paradigm is, that the ionic electronics on the liquid 'cellular' side is capacitive decoupled for the solid semiconductor electronic side of the CMOS chip. Here the dielectric interface is of ultimate importance and several approaches and material combinations were reported to optimize the material in contact to the cells.

Conductive polymers, where poly(3,4-ethylenedioxythiophene) doped with polystyrene sulfonate (PEDOT:PSS) is the most prominent candidate, carry the electrical current in a fundamentally different way compared to silicon. The electrical conductivity in this polymer matrix can be modulated by doping and de-doping with cations from the liquid, which offers the possibility to engineer organic electrochemically gated transistors (OECTs). When the material is over-oxidized, the electronic conductivity is suppressed and only the ionic conductivity remains. This has been demonstrated to enable ionic pumps, where the ion conductor functionality can be used to locally administer chemicals and drugs.

In this presentation, several microsystems and applications will be discussed, where a combination of silicon-based electronics with organic polymer electronics is enabling novel functionality. Thereby combinations of inorganic/organic materials integrated in various transistor array types are used to interface cells and tissue^{1,2}. Several examples developed in the clean room facilities of IWE1 at RWTH Aachen University will be discussed, where we aim towards multi-modal bioelectronics communication including electrical as well as biochemical sensing and actuation principles.

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Figure: Example of a long-term test platform for the observation of epileptical activity in mouse brain slices¹. The sensors are integrated on a flexible substrate while a coating of PEDOT:PSS enables a low input impedance and hence a high signal-to-noise ratio.

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Quantitative Analogue Simulation of Planar Molecules

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Abstract

Synthetic quantum systems provide a pathway for exploring the physics of complex quantum matter in a programmable fashion. This approach becomes particularly advantageous when it comes to systems that are thermodynamically unfavorable. By sculpting the potential landscape of Cu(111) surfaces with carbon monoxide quantum corrals in a cryogenic scanning tunneling microscope, we created analogue simulators of planar organic molecules, including antiaromatic and non-Kekulé species that are generally reactive or unstable. Spectroscopic imaging of such synthetic molecules reveals close replications of molecular orbitals obtained from ab-initio calculations of the organic molecules. We further illustrate the quantitative nature of such analogue simulators by faithful extraction of bond orders and global aromaticity indices, which are otherwise technically daunting using real molecules. Our approach therefore sets the stage for new research frontiers pertaining to the quantum physics and chemistry of designer nanostructures.

Metal-organic framework membrane for harvesting osmotic energy

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Abstract

Metal-organic framework (MOF) membranes that replicate ion channels enable the development of groundbreaking separation technologies and energy-harvesting devices by achieving high selectivity and osmotic power generation, opening up new possibilities previously unmapped. In particular, nanometrically thin uniform MOF membranes are capable of remarkably high osmotic power generation. Propelled by osmosis, MOFs exhibit an extraordinary selectivity with remarkable features that enable them to generate an unparalleled power output when subjected to salt gradients such as sea-river water boundaries[1]. Here we are presenting the synthesis of a tunable-thickness metal catecholate (MOF) with a very high osmotic power output of 100s of W/m². A Liquid-liquid interfacial synthesis method of free-standing MOF is followed, which has very good control over their thickness by varying concentration of composition materials and reaction time. Free-standing MOF can be transferred onto any substrate which is convenient for analytical measurements. This facile method and large-scale synthesis capability uphold scalability for practical applications.

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Coexistence of Superconductivity and Chiral Charge Density Wave in TiSe₂

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Abstract

Chirality breaks down the inversion symmetry and results in unexpected new electronic properties in systems with reduced dimensionality. Stark examples of manifestation of chirality on electronic properties of materials are carbon nanotubes - the conductivity ranges from insulating to superconducting dependent on the structural chirality of the nanotubes. In addition to structural chirality, the chiral state can also manifest itself in the arrangement of electronic states – magnetic vortices, skyrmions, chiral superconductors. TiSe₂ is the first known material that exhibits chiral charge density wave state.

TiSe₂ is a member of transition metal dichalcogenide family of layered van der Waals materials that has attracted significant interest due to the intricate mechanism that drives its transition from a semiconducting to a charge density wave (CDW) phase. The unique chiral character of the CDW in TiSe₂, is complemented by several exciting features that are associated with this particular material. First, the CDW in 1T–TiSe₂ is induced by combination of excitonic instability, Jahn-Teller effect, and electron-phonon coupling. This opens plethora of opportunities for manipulating the CDW state using light.

We demonstrate the chiral properties of the CDW through several independent techniques: scanning probe microscopy, transient optical reflectivity and photogalvanic effect. As temperature is decreased below $T_{CDW}=200 \text{ K}$ 1T-TiSe₂ goes first from the high temperature normal phase to a $2 \times 2 \times 2$ achiral CDW phase at T_{CDW} and then to a chiral phase at T_{ch} . These two thermodynamic transitions were first observed using bulk thermodynamic techniques [1], and their nature explored in more detail using photogalvanic effect [2]. The structure of the chiral CDW was imaged using scanning tunneling microscopy[3], while time-resolved optical reflectivity and IR studies clearly show that the chiral order can be non-thermally melted and controlled using circularly polarized light.

Our study provides compelling evidence for the spontaneous emergence of chirality in the correlated semimetal TiSe₂. Such chiral induction provides a new way of optical control over novel orders in quantum materials and potential for novel electrooptical sensing.

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Protein Nanopores: From Lethal Toxins to Chemical, Polymer, DNA, & Protein Analysis at the Single Molecule Level

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Abstract

The most well-known nanometer-scale protein nanopores (i.e., ion channels) provide the molecular basis of mammalian nerve and muscle activity. In a twist on their function, we adapted single protein nanopores to accurately determine the physical-chemical properties of individual molecules. Over the past three decades, the technique has been used in a wide range of applications including quantifying ion concentrations, discriminating between polymers based on their size, and sequencing DNA via two independent methods. I will describe what made the method possible and show how it is currently being developed to identify proteins, including point mutations and post-translational modifications. In addition, I will discuss what limits our understanding of lethal anthrax-induced infection facilitated by the bacterial pore-forming toxin *Bacillus anthracis* Protective Antigen.

Photoluminescence enchantement in monolayer transition metal dichalcolgenides

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Abstract

Excitons in monolayer transition metal dichalcogenides (TMDCs) present fascinating opportunities for optoelectronics, distinct from those found in bulk semiconductors. However, intrinsic defects within TMDCs hinder the radiative recombination pathways of excitons, leading to limited photoluminescence (PL) quantum efficiency. Various methods, such as superacid treatment, electrical doping, and plasmonic engineering, have been explored to suppress nonradiative decay channels and enhance PL intensity. Here, I will introduce a more straightforward approach to enhance PL quantum efficiency. By creating metal-semiconductor heterojunctions, we observe a remarkable increase in PL intensity—up to an order of magnitude— at technologically relevant excitation powers. The findings I will present shed light on metal-semiconductor interactions and offer a promising path for large-scale integration-compatible improvements in the optoelectronic performance of semiconducting TMDCs. [1]

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Nanoscale mass transport in 2D and 1D nanomaterials

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Abstract

2D and 1D nanomaterials present ideal model systems to probe nanoscale mass transport phenomena at extremes of length scales. In this talk, I will discuss our recent results on the synthesis of 2D and 1D nanomaterials, subsequent fabrication of membranes by incorporating the nanomaterials, and studying the transport of model molecules for separation applications.

Specifically, I will discuss molecular sieving and ultra-low friction transport in wafer-scale carbon nanotube (~0.5-4.5 nm) capillary membranes. Our CNT membranes offer advantages of significantly higher hydraulic permeability, greatly enhance removal of middle molecules and comparable albumin retention to overcome persistent challenges in hemofiltration. Finally, I will introduce new approaches to heal defects in atomically thin membranes by leveraging a new class of biomolecules and transport through 1D and 2D nanomaterials for biological separation applications including dialysis and beyond.

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Controlling charge-density wave states in monolayer TiSe₂

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Abstract

Control over materials thickness down to the single-atom scale has emerged as a powerful tuning parameter for manipulating not only the single-particle band structures of solids, but increasingly also their interacting electronic states and phases. A particularly attractive materials system in which to explore this is the transition-metal dichalcogenides (TMDs), both because of their naturally-layered van der Waals structures and the wide variety of materials properties which they are known to host. Here, I will discuss our work integrating monolayer materials growth by molecular-beam epitaxy with electronic structure studies via *in situ* angle-resolved photoemission and ARPES-based microscopy. I will introduce a new growth approach which leads to a step-change in the quality and uniformity of the growth of our TMD monolayers [1]. This, in turn, opens the door to the fabrication of epitaxial van der Waals heterostructures, including samples fabricated via hybrid exfoliation-epitaxy approaches. I will discuss the resulting electronic structure in these systems, with a focus on TiSe₂, and will investigate how its charge density wave order varies with chemical substitution, charge doping, and control of the dielectric screening [2-5], providing insights into the nature of the controversial phase transition in this system.

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Beam search decoder for enhancing sequence decoding speed in single-molecule peptide sequencing data

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Abstract

Next-generation single-molecule protein sequencing technologies have the potential to significantly accelerate biomedical research. These technologies offer sensitivity and scalability for proteomic analysis. One auspicious method is fluorosequencing, which involves: cutting naturalized proteins into peptides, attaching fluorophores to specific amino acids, and observing variations in light intensity as one amino acid is removed at a time. The original peptide is classified from the sequence of light-intensity reads, and proteins can subsequently be recognized with this information. The amino acid step removal is achieved by attaching the peptides to a wall on the C-terminal and using a process called Edman Degradation to remove an amino acid from the N-Terminal. Even though a framework (Whatprot) has been proposed [1] for the peptide classification task, processing times remain restrictive due to the massively parallel data acquisicion system. In this paper, we propose a new beam search decoder with a novel state formulation that obtains considerably lower processing times at the expense of only a slight accuracy drop compared to Whatprot. Furthermore, we explore how our novel state formulation may lead to even faster decoders in the future.

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Exciton Manipulation and Transport in 2D Semiconductor Heterostructures

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Abstract

Long-lived interlayer excitons in van der Waals heterostructures based on TMDCs have recently emerged as a promising platform for controlling exciton transport on the mesoscopic length scales, allowing control over exciton diffusion length, energy and polarization. One of the driving forces for exciton transport is the interaction between out-of-plane dipoles in the exciton bosonic gas. By using spatial and time-resolved photoluminescence imaging, we can observe the dynamics of exciton transport, enabling a direct estimation of the exciton mobility [1]. The presence of interactions significantly modifies the diffusive transport of excitons, effectively acting as a source of drift force and enhancing the diffusion coefficient by one order of magnitude. In certain types of vdW heterostructures, the layer hybridization and exciton-exciton interaction can also be electrically tuned, allowing us to uncover dipole-dependent properties and transport of excitons with different degrees of hybridization [2]. Moreover, we find constant emission quantum yields of the transporting species as a function of excitation power with dominating radiative decay mechanisms dominating over nonradiative ones, a fundamental requirement for efficient excitonic devices.

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Magnetoelectric phenomena of noncentrosymmetric superconductors

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Abstract

Superconductivity in materials with broken inversion symmetry has been a subject of theoretical and experimental studies from the early 90's. It was understood that unlike symmetric spin-orbit coupling found in centrosymmetric metals, spin-orbit coupling in non-centrosymmetric materials has a spectacular influence on the electronic bands through a specific spin splitting of the quasiparticle states. Superconductivity as a Fermi-surface instability towards pairing of electrons with opposite momenta and spins is naturally influenced by such a modification of the electronic states. The removal of inversion symmetry and also of time-reversal, e.g. by an applied external magnetic field, promotes a novel form of electron pairing-the so-called helical phase, in which Cooper pairs acquire a finite center of mass momentum. The latter gives rise to several interesting magneto-electric or magneto-chiral effects, like the enhancement of T_c in the presence of magnetic fields, the supercurrent diode effect, magneto-chiral inductance anisotropy, zero-pilike transitions, the anomalous Josephson effect, as well as, unusual vortex squeezing and engendered London physics in the Meissner state. The last decade witnessed a renewed interest in superconductors with broken inversion symmetry by using the so-called synthetic superconductors, e.g. 2DEG with a strong Rashba spin-orbit-coupling in a proximity of conventional superconductors, in a pursuit to find or engineer topologically non-trivial superconducting states with non-Abelian (Majorana) excitations.

In the talk I will discuss general properties of the non-centrosymmetric superconductors summarizing the main theoretical and phenomenological concepts standing behind. Apart of that, I will present exciting experimental evidences showing the emergence of i) *supercurrent diode effect* and *Josephson inductance anisotropy* [1] in the synthetic Josephson junctions incorporating proximitized 2DEG formed in InAs-quantum wells that possess strong Rashba coupling and large g-factor, ii) *zero-pi-like transitions* and *anomalous Josephson effect* [2] in such non-centrosymmetric systems, and, last but not least, also iii) an *unexpected enhancement of pinning and squeezing* of Abrikosov vortices when probed in such Rashba-based superconductors in a Meissner phase [3]. I will elucidate these phenomena from the microscopic point of view, but as well as, phenomenologically–as a direct manifestation of the Lifshitz invariant that is allowed in the Ginzburg-Landau free energy when the underlying Cooper pairs acquire a finite center of mass momentum.

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Figure 1. a, Sample inductance of Rashba superconductor as a function of in-plane magnetic field for different orientations of the driving current (red and blue symbols). The controlled measurement (grey symbols) corresponds to a centrosymmetric (i.e. non-Rashba) superconductor. b, Polar plot showing the angle dependence of the vortex inductance for selected values of out-of-plane magnetic field. c, The color

plot schematically represents the modulus of the order parameter, $|\psi(x,y)|^2$, near the core of a pinned vortex, in the absence of in-plane field. The horizontal black arrow represents the direction of a current bias, while the white arrow indicates the direction at which a Lorentz force acts on a pinned vortex. The measured vortex inductance is rotation symmetric and inversely proportional to the curvature of $|\psi(x,y)|^2$ along the force direction. d-f, When a finite in-plane field is applied the vortex core is squeezed as a consequence of the Rashba spin-orbit interaction, reflecting the measured change in vortex inductance. The curvature is always probed along the white axis, rotating the in-plane magnetic field the vortex rotates keeping its small elliptic axis parallel with the direction of in-plane field. This allows one to extract from the vortex inductance the spatial profile –order parameter tomography--of $|\psi(x,y)|^2$.

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Graphene- and hexagonal boron-nitride-based in-vitro cell-culturing surfaces beneficially influence the spatial distribution of neonatal spiral ganglion neurons

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Abstract

Neural interfaces based on novel graphene-based materials address limitations of low spatial resolution and broad specificity of neuronal stimulation in current cochlear implant devices leading to poor pitch perception and significant variability in its efficacy. Graphene and other two-dimensional (2D) materials possess several properties (flexibility, electrical mobility, large surface area, biocompatibility compliance), making them attractive for implementation in next-generation cochlear implants. Graphene was shown to support neural growth due to its unique electric properties, biocompatibility with neuronal cells, and capacity to interface with neuronal tissue effectively [1]. In addition, recent studies of hexagonal boron nitride (hBN) showed promising applications in neuroengineering due to its high stability, processability, parameter tunability, and biocompatibility [2]. However, it is yet unknown how graphene and hBN affect the cellular morphology of spiral ganglion neurons (SGN).

In this study, three types of graphene-based substrates (single-layer graphene - SLG, hydrogenated graphene - HG, and fluorinated graphene - FG), along with a single-layer hexagonal boron nitride (SLhBN), were utilized as surface layers on which in-vitro cultures of neonatal SGNs extracted from rat pups were seeded and cultured. We stained these cultures immunocytochemically at eight days in vitro (8DIV) and subsequently analyzed fluorescence images with custom-made machine learning-based image processing allowing automatic identification and segmentation of neurons. We identified several morphological parameters related to the spatial distribution of SGNs grown on experimental 2D surfaces and compared them with those grown on glass coverslips. Analysis with the mixed effect model revealed that SLG, HG, and SLhBN, but not FG substrates represented a more favorable environment for SGNs growth, resulting in significantly altered spatial distribution compared with those SGNs grown on control coverslips.

The obtained results confirm graphene as a material suitable for the growth and development of SGN and its potential application in devices such as cochlear implants. Furthermore, these findings reveal new knowledge about graphene- and hBN-based substrates' influence on the growth and development of in-vitro SGN cell cultures.

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Pressure-induced topological phase transition in ZrTe₅

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Abstract

Zirconium pentatelluride (ZrTe₅) is a novel candidate topological insulator (TI) that, when grown using chemical vapor transport (CVT) techniques, appears to be in the weak TI phase in ambient conditions, but close to the topological phase transition to strong TI.^[1] In addition, its band structure is highly sensitive to small changes in lattice constants.^[2] Using a recently developed method for studying nanodevices under hydrostatic pressure,^[3] we perform detailed magnetotransport measurements on ZrTe₅ devices at different pressures. Applying a multicarrier transport model to obtain band structure information, the results show a closing and subsequent re-opening of the direct gap at the Γ point with application of pressure, being an indication of passing through the phase transition from weak to strong TI.^[4] This is shown to be consistent with expectations from *ab initio* band structure calculations, as well as previous observations that CVTgrown ZrTe₅ is in a weak topological phase in ambient conditions.

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TWISTED LIGHT CONTROL OF FERROELECTRIC ORDER IN A RASHBA-TYPE SEMICONDUCTOR

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Twisted light, i.e. light beams which possess field gradients forming an optical vortex, possess a measure of orbital angular momentum that can be transferred from light to electrons [1]. The interplay between twisted light with dipolar systems in condensed matter has been scarcely explored, especially in systems with abundant forms of topologies such as skyrmions, or systems which embrace strong light-matter coupling such as ferroelectrics. An optical vortex beam has a phase singularity with a certain topological charge, giving rise to a hollow intensity distribution. Such a beam with helical phase fronts and orbital angular momentum was predicted to be imprinted coherently in ferroelectrics as a transient electrodynamical response of the optical vortex [2]. Recently optical-vortex interactions in condensed-matter expanded also to Rashbatype spin-orbit interaction, suggesting selection rules that lead to coupling between the light's orbital and matter spin-angular momentum [3]. In this regard α -GeTe offers an interesting testbed for twisted light interaction with ferroelectric order, in which the combination of the ferroelectric order and large spin-orbit interaction yields in a switchable Rashba-type spin structure of the bulk states [4]. Our x-ray standing wave experiment from a 5 nm thick α -GeTe film grown on InP(111) and $BaF_2(111)$ substrates provides a direct evidence of such a light-matter interaction showing coherent poling of the Ge-Te bonds upon OAM with various topological charges, consistent with the applied bias. The topological charge ± 1 and ± 3 of the optical vortex was generated with spiral zone-plates. To further corroborate our experimental results, by changing the OAM we present NEXAFS data showing energy shifts of the Ge-K edge due to chemical shifts associated with the Ge-Te poling, accompanied by pronounced dichroism of the Ge-K edge upon OAM Supported by state-of-the art scattering calculations of the NEXAFS spectra, our results change. indicate all-optical control of the α -GeTe ferroelectricity with OAM light, which does not suffer from limitations associated with the requirement of circuitry access with ferroelectric manipulation via applied bias. Besides this, our results indicate that the ferroelectric poling in α -GeTe is supporting the long-sought evidence of the order-disorder ferroelectric polarization mechanism.

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The electro-solvation force: a new paradigm in soft matter and biology

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Abstract

The interaction between charged objects in solution is generally expected to recapitulate two central principles of electromagnetics: (1) like-charged objects repel, and (2) they do so regardless of the sign of their electrical charge. We have demonstrated experimentally that the solvent plays a hitherto unforeseen but crucial role in interparticle interactions, and importantly, that interactions in the fluid phase can break charge-reversal symmetry [1]. We have shown that in aqueous solution, negatively charged particles can attract at long range while positively charged particles repel. In solvents that exhibit an inversion of the net molecular dipole at an interface, such as alcohols, we find that the converse can be true: positively charged particles may attract whereas negatives repel. The observations hold across a wide variety of surface chemistries: from inorganic silica and polymeric particles to polyelectrolyte- and polypeptide-coated surfaces in aqueous solution. A theory of interparticle interactions that invokes solvent structuring at an interface captures the observations. Our study establishes a nanoscopic interfacial mechanism by which solvent molecules may give rise to a strong and long-ranged force in solution, with immediate ramifications for a range of particulate and molecular processes across length scales such as self-assembly, gelation and crystallization, biomolecular condensation, coacervation, and phase segregation.

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Quantum Transport Equations in heavily doped graphene: Self-Consistent RPA Approach

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Abstract

The generalized Drude approach represents a model-independent method of analyzing measured reflectivity spectra. [1] In this approach, the dynamical conductivity formula is given in terms of a phenomenological frequency-dependent memory function. The same expression for the dynamical conductivity can be obtained theoretically by using different types of quantum transport equations. Here, we present the results for the memory-function dynamical conductivity in weakly and heavily doped graphene obtained by using a common self-consistent RPA approach. [2,3] We will show that a seemingly inconsistent dependence of the dc conductivity of ultraclean and dirty lightly doped samples on doping can be easily understood if in the calculations the momentum distribution functions are used instead of the Fermi-Dirac distribution functions. [4] We will also show that the redistribution of the intraband conductivity spectral weight over a wide frequency range, clearly seen in experiments, can be explained by replacing the intraband relaxation rate by the corresponding intraband memory function. For the scattering of conduction depend on frequency and temperature in the way shown in Fig.1(a). [3] Fig.1(b) illustrates the corresponding infrared conductivity.



Figure 1. (a) The real and imaginary parts of the phonon contribution to the memory function in heavily doped graphene, for typical values of model parameters. (b) The corresponding infrared conductivity.

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Tomographic active matter

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Abstract

Over the last few decades, electrical engineers, physicists and chemists have put considerable efforts into designing self-propelled micro robots with the dream to revolutionize microsurgery, safety and exploration in extreme and severe conditions. As soon as it approaches the true microscale, these robots lose their ability to carry a camera, whether due to the intrinsic diffraction limit or the limited on-board computing power. These robots would essentially be blind and unable to access their orientation. So, it is surprising that these robots, though technologically elegant, would be of any practical use.

In this talk, I will introduce a new mathematical result that enables these robots to recognize shapes. We carried out a simple proof-of-concept with a toy commercial robot known for its exceptional pedagogical appeal, and showed that a robot lacking visualization or internal compass capabilities can perform autonomous pattern recognition. We also show that this new mathematical theorem enables the robot to read letters and words.



Figure 1. Example of possible recognized patterns (pictures adapted from [1])

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Probing the Itinerant Magnetic Behavior of FeRh using In-situ Electron Magnetic Circular Dichroism (EMCD)

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Abstract

EMCD is an electron microscopy approach, analogous to X-ray magnetic circular dichroism (XMCD), that provides spatially resolved and element-specific information about spin and orbital magnetic moments. Though dynamical electron scattering effects and microscope aberrations make EMCD measurements more complex to execute than XMCD, EMCD can have spatial resolution orders of magnitude higher down to atomic scale. Such a spatial resolution allows assessing the fundamental aspects of what magnetism probe actually sense. In particular, questions arise in the quantitative interpretation of dichroic signals in different types of magnets having itinerant or local moments when the probe size is smaller than the wavelength of spin fluctuations and collective spin dynamics. To explore these fundamental aspects, we studied FeRh, an itinerant magnet. Exploiting the first-order transition from antiferromagnetic (AFM) to the ferromagnetic (FM) phase in FeRh as a reference for quantitative ECMD, we show that the measured spin-orbital magnetic moments differ by an order of magnetic between 1µm and 0.2 nm probes. Considering the deep microscopic meaning of what a local moment is and its relation to the concept of valence, it can be argued that a high-energy probe, such as in EMCD and XMCD measurements, are inherently fast. Thus, we suppose these fast probes take snapshots of the local moments in the presence of a deep core-hole that de facto momentarily quenches the valence fluctuations due to nature of metallic bonding, exposing the instantaneous local moment on the ion. The question then arises: what probe size is required for meaningful measurements, i.e., how should it relate to the wavelength of collective fluctuations? By studying the influence probe size on the ml/ms orbit-spin moment ratio, we hope to shed light on fundamental aspects of how we interpret XMCD and EMCD spectroscopy data.
Investigation of Abrikosov vortex phases in defect-engineered copper-oxide superconductors

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Abstract

The study of how strategically placed topological defects influence the distribution of Abrikosov vortices in a superconductor hinges on the precise creation of a vortex-pinning potential landscape. It is essential to magnetically couple these vortices, ensuring their separation does not exceed the London penetration depth at the target operating temperature. This temperature must be substantially below the superconductor's critical temperature T_c to mitigate the effects of thermodynamic fluctuations. Achieving the necessary nanoscale precision is particularly challenging in copper-oxide superconductors due to their intricate atomic structure and sensitivity to environmental factors. Traditional lithographic methods face significant limitations in this context, but these can be circumvented by employing the focused beam of a helium ion microscope (He-FIB). The 30 keV He⁺ ion beam is utilized to create hexagonal arrays of defect columns in thin films of YBa₂Cu₃O_{7- δ} and square arrays in Bi₂Sr₂CaCu₂O_{8+x}. Within these nanocolumns, T_c is suppressed due to pair-breaking caused by numerous point defects.

The unique topology of our pinning landscapes results in several notable phenomena. We observe vortex commensurability effects at high magnetic fields, reaching up to 6 T [1]. The interplay between vortex pinning at regular and intrinsic irregular sites leads to the formation of an ordered Bose glass of vortices [2,3]. Moreover, we observe reentrant zero resistance at an applied magnetic field of 3.8 T, accompanied by a pronounced peak in the pinning force density of the vortex ensemble. When the vortex density aligns with the precisely known density of defect columns, the observation of commensurability effects enables us to determine the pinning force exerted on a single vortex by an artificial defect. We will also discuss how this pinning force varies with temperature.

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Phonon anomalies and pressure temperature phase diagram of CsV₃Sb₅

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Abstract

The recent discovery layered Kagome superconductors AV3Sb5 (A=K, Cs, Rb) has sparked considerable excitement. These materials are characterized by an electronic structure featuring flat bands, van Hove singularities (vHs), Dirac cones, and non-trivial band topology, and offer a unique platform for exploring novel electronic states of matter with intertwined orders. At temperatures well above their superconducting Tc (2,7K in CsV3Sb5), an electronic superlattice commonly associated with a CDW. To date, no Kohn-anomalies associated with the formation of this CDW have been observed in their phonon dispersion, whereas chirality, time-reversal symmetry breaking or electronic nematicity have been reported, indicating that the underlying electronic order might be substantially more complex. High pressure studies have revealed a double superconducting dome structure associated with the changes in the nature and disappearance of the CDW inferred from indirect measurements.

I will present a detailed high pressure x-ray diffraction study of these materials showing in detail how the lattice superstructures evolve across the phase diagram. Previously unreported anomalies in the lattice dynamics across the CDW formation will also be presented. These results bring novel insights on the nature and origin of the CDW, challenging in particular scenario in which it arises from a Peierls-like nesting of occupied van Hove Singularities.

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Electron-Ion Interaction in 2D Semiconductor Nano-Fluidics.

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Abstract

We investigate the interaction between ions flowing through sub-nanometer pores in 2D semiconductor materials such as graphene and transition metal dichalcogenides (TMD), and their electronic environment. We pay special attention to so-called 2D "Janus" layers such as MoSSe, where the charge imbalance between sulfur and selenium atoms on each side of the atomic molybdenum layer creates an asymmetry in the ionic current. Our methodology integrates molecular dynamics simulations with Boltzmann transport formalism to study the ion and electron dynamics influenced by electrical and steric interactions in solid-state membranes.

We discuss the potential of semiconductor nanoscale channels to achieve electronic Coulomb drag by flowing ions as a versatile process for blue energy harvest, for which we predict current amplification as a consequence of interaction between heavy ions and light electronic particles, and address design optimization of the 2D channels for Coulomb drag enhancement.



Figure1: Snapshots of the two-step ion transport through a 0.8nm-diameter "Janus" MoSSe nanopore with corresponding timestamps under 1 V forward bias.

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Nanopore elastometry of biological nanostructures

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Abstract

Studying the mechanical properties of small biological nanoparticles, typically below 100 nm in size, provides valuable insights into their structural characteristics and functional mechanisms^[1]. However, current techniques characterizing nanomechanical properties of individual particles, such as nanoindentation, atomic force microscopy, optical tweezers, etc., are hampered by complex procedures and limited throughput, thereby constraining their broader application^[2]. In this study, we introduce a new, efficient method: nanopore squeezing, involving electrophoretic pulling of soft particles through smaller nanopores while monitoring the corresponding ionic current blockage. As a proof of concept, we investigate the squeezing behavior of 3D wireframe DNA nanoparticles (DNA-NPs), liposomes, and polymersomes through nanopores of varying diameters, ranging from 8 to 100 nm. We discovered three distinctive translocation regimes: (1) Random-activated Regime: DNA-NPs translocate slowly through the nanopore due to creep deformation of the overall wireframe structure at low voltages, with translocation speed exhibiting weak voltage scaling. (2) Friction Regime: DNA-NPs rapidly collapse and pass the nanopore at high voltages, with a linear increase in speed corresponding to voltage maintaining constant constraint mobility. (3) Transition Regime: this regime marks a transition between the two aforementioned translocation mechanisms, occurring at an onset voltage. For liposomes and polymersomes, we observed two primary signal types: Spike-shaped events and friction events. The occurrence rate of the latter increases superlinearly with voltage, and it is correlated with poration of the membrane material. This new method has promising applications in diagnostics, particularly for identifying and characterizing viruses, exosomes, and other biological nanoparticles, advancing our understanding of these essential biological entities.

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Towards electrochemical functionalization of 2D materials for nanosensing devices

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Abstract

Surface functionalization and nanostructuring of two-dimensional (2D) materials open possibilities for creating new hybrid materials and nanoarchitectures. Attaching different molecules onto the surface of 2D transition metal dichalcogenides (TMDCs) can be used to tune their optoelectronic and catalytic properties, surface charge and surface chemistry, but also bring new functionalities that could be harnessed in a new generation of nanodevices. Tailoring surface chemistry is particularly beneficial for devices, such as nanofluidic and (bio)sensing devices, that are operating in liquid or strongly interacting with chemical species [1,2].

Due to chemical inertness of TMDC's basal plane, the surface functionalization is typically limited to TMDC's defective sites, often requiring conversion of the TMDC from its semiconducting into metallic phase. Electrochemical methods have the advantage of utilizing the voltage applied to 2D material to initiate and drive the chemical reaction, thus introducing an active control during surface functionalization process [3,4].

In our work, we used electrochemical approach for modifying the basal plane of 2D molybdenum disulfide (MoS₂). Our method employs electrografting of aryl-diazonium salt, 3,5-bis(trifluoromethyl)benzenediazonium tetrafluoroborate, resulting in uniform surface coverage without the need for pre-existing defects or phase transition. Furthermore, we demonstrate the advantage of this approach by selectively addressing individual MoS₂ nanoribbons via different electrodes thus achieving highly selective functionalization at the nanoscale. The ability to selectively address individually contacted 2D layers opens the possibility for specific surface modification of neighboring 2D nanostructures by different functional groups leading towards advanced functionality and performance of future nanodevices.

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Non-reciprocal phase transitions

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Abstract

Spontaneous synchronization is at the core of many natural phenomena. Your heartbeat is maintained because cells contract in a synchronous wave; some bird species synchronize their motion into flocks; quantum synchronization is responsible for laser action and superconductivity. The transition to synchrony, or between states of different patterns of synchrony, is a dynamical phase transition that has much in common with conventional phase transitions of state – for example solid to liquid, or magnetism – but the striking feature of driven dynamical systems is that the components are "active". Consequently quantum systems with dissipation and decay are described by non-Hermitian Hamiltonians, and active matter can abandon Newton's third law and have non-reciprocal interactions. This substantially changes the character of many-degree-of-freedom dynamical phase transitions between steady states and the critical phenomena in their vicinity, since the critical point is an "exceptional point" where eigenvalues become degenerate and eigenvectors coalesce.

We will illustrate this in several different systems – a Bose-Einstein condensate of polaritons, models of multicomponent active matter such as flocks of birds, generalized Kuramoto models, and others. We argue that there is a systematic theory and generalized phase diagram, and corresponding universality behaviors determined by the symmetry of the models.

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Electronic quantum transport simulation for 2D materials

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Abstract

Over the past two decades since the discovery of the very first two-dimensional (2D) material: graphene, quantum transport simulation based on the real-space Green's function method within the Landauer-Büttiker framework has shown its power in reproducing and predicting low-temperature transport measurement in the clean limit. This talk starts with a brief introduction to the formalism, and then illustrates a few examples of simulating electronic transport in cleans samples, possibly including graphene, strained graphene, bilayer graphene, MoS₂, and so on. Extra attention will be paid to two of our latest works: Transverse magnetic focusing in graphene proximitized with strong spin-orbit coupling by WSe₂ [1] and the four-band effective square lattice model for Bernal-stacked bilayer graphene [2]. The former reported a record-breaking spin-orbit coupling strength of about 13 meV from the transport experiment, which was qualitatively reproduced by our spin-dependent transport simulation, while the latter allows for micron-sized two-dimensional transport in bilayer graphene.

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The optical response of the quantum material family BaCoS₂-BaNiS₂

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Abstract

 $BaCoS_2$ and $BaNiS_2$ are the end members of a solid solution that shows a vast array of quantum properties. The Co material is a strongly correlated insulator with an antiferromagnetic transition, as well as a structural phase transition, around room temperature. At 28% Ni doping the solution undergoes an electronic metal-insulator phase transition to a Drude metal. The metallicity persists all the way to the pure Ni compound, where in addition to the Drude metal, we observe a strong contribution from bands with linear dispersion at the Fermi level. These will give origin to dispersive Dirac nodal lines. We performed optical conductivity measurements combined with ab-initio calculations to reverse engineer the role of each band in the physical response of these materials. We explained uncommon features in their optical response such as a linear dispersion of the optical conductivity [1] and the existence of an isosbestic line separating a spectral-weight transfer across Dirac nodal states [2].

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Soft-mode superconductivity in incipient ferroelectrics

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Abstract

SrTiO3 (STO) and KTaO3 (KTO) are known for their proximity to a ferroelectric phase. STO shows bulk superconductivity with a characteristic domelike behavior resembling systems close to a quantum critical point. Several mechanisms have been proposed to link these phenomena, but the abundance of undetermined parameters prevents a definite assessment. We show that a Rashba-type one-phonon spin-orbit-assisted coupling [1] can explain the magnitude of the critical temperature and the dome-like behavior in STO (see Figure). The dome is attributed to a momentum-dependent quenching of the angular momentum due to a competition between spin-orbit and hopping energies. The optimum density for having maximum Tc results in good agreement with experiments without free parameters. These results make the generalized Rashba dynamic coupling to the ferroelectric soft mode a compelling pairing mechanism to understand bulk superconductivity in doped STO. We also discuss the prospect of this mechanism in KTO where spin-orbit interaction effects are even larger [2].



Figure 1. Tc dome (normalized to its maximum value) vs. carrier density. The full (dashed) line neglects (includes) the hardening of the TO mode with density. Open symbols are bulk T_c experimental data from Koonce, PRB 1967 (circles), Collignon, PRB 2017 (triangles) and Thiemann, PRL 2018 (diamonds) using

 $T_{c,max} = 0.35K$. Inset: band resolved electron phonon coupling, λ_{BCS} using the abinitio results.

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Nanoscale maps and field effects in proton transport through 2D crystals

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Abstract

Graphene, a one-atom-thick sheet of carbon atoms, is completely impermeable to all atoms – even helium, the smallest – under ambient conditions. Nevertheless, it is permeable to thermal protons [1]. This finding opened a debate on whether the proton permeability was due to vacancies, which remained in stalemate for almost a decade. In this talk we'll discuss our recent work mapping proton transport currents in graphene with nanoscale spatial resolution, which confirm that perfect graphene crystals are permeable to protons [2]. We have also found that the same holds for the disordered material graphene oxide, albeit only under small scale areas [3]. We will also discuss our recent work investigating the role of electric field effects in accelerating proton transport and proton adsorption (hydrogenation) on graphene [4]. Using a technique known as double gating, we demonstrated that these otherwise coupled processes can be controlled independently, enabling proton-based logic and memory applications.

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Scanning Tunneling Microscopy of Twisted 2D Semiconductors

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Abstract

Twisting bilayers of transition metal dichalcogenides gives rise to moiré potentials responsible for novel ferroelectricity or correlation effects. In this talk, I will focus on STM/STS experiments on twisted WS₂ both in the parallel and antiparallel regimes.

In marginally twisted samples, we show that by tuning the electric field under a scanning tunneling microscope, one can achieve local control of the ferroelectric domains at room temperature. We discuss their reversible evolution using a string-like model of the domain wall network. In the case of antiparallel alignment, we reveal localized states in the vicinity of the valence band onset and by comparison to theory we understand the role of out-of-plane relaxation on the reconstructed band structure.

Lastly, I will discuss new results on twisted graphene multilayer in a helical arrangement.



Figure 1. Scanning Tunneling Microscopy of Twisted Semiconductors

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Using uniaxial pressure to both tune and probe quantum materials

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Abstract

In this talk I will discuss rapid developments in applying uniaxial pressure to quantum materials using piezo-activated vices. In the first stages of using the new experimental capabilities, the focus was on applying large static uniaxial pressures, to generate large changes in the physical properties of unconventional superconductors and magnets. The vice provided the tuning of the properties, which were probed by other techniques such as electrical resistivity or magnetic susceptibility. Only more recently has it become clear that exquisitely precise thermodynamic information can be obtained from simultaneously probing the elastic response of the materials to the applied pressure. These new techniques rely on combining static pressure with a tiny oscillatory component, and locking in to the responses of the material at the frequency of those oscillations. They are enabled only via the basic strategy of applying the pressure using piezoelectric actuators. In my opinion an entirely new avenue of quantum materials research can be opened with this new combination of tuning and measurement, as I will attempt to explain.

Optical trapping microscopy as a probe for nonequilibrium physics

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Abstract

We propose optical trapping microscopy as a probe for nonequilibrium physics. Optical trapping microscopy enables the direct observation of Maxwell-Boltzmann distributions. Changes in this the distribution are measurable over length scales comparable to the trapped particle's size and on time scales limited by the resolution of the experimental setup. Possible physical systems to test optical trapping microscopy as a probe of nonequilibrium physics are discussed.

Vortex-core states and conductance modulations revealed in Bi₂Sr₂CaCu₂O_{8+δ} with Scanning Tunneling Spectroscopy

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Abstract

The electronic structure of the Abrikosov vortices is one of the outstanding puzzles of high temperature superconductivity (HTS) [1]. For long, vortices explored with Scanning Tunneling Microscopy in HTS cuprates were systematically lacking the electronic signatures predicted by Wang and MacDonald for *d*-wave superconductors [2]. It is only recently that the zero-bias conductance peak expected at the center of the flux lines was observed in heavily-overdoped $Bi_2Sr_2CaCu_2O_{8+\delta}$ (Bi-2212) single crystals measured at an unprecedented low magnetic field [3]. These experiments also confirmed our earlier findings that other cuprates like YBa₂Cu₃O_{7-x} can also host conventional *d*-wave vortex cores [4]. However, other vortex cores measured in Bi-2212 in similar regimes still reveal the unusual electronic features reported previously, including the periodic conductance modulations in the vortex halos and low energy subgap states.

Our recent measurements investigate how these electronic states and charge orders evolve as a function of various experimental parameters, shedding new light on the debated links between the sub-gap states, the checkerboard patterns, the vortex core conductance peak and the pseudogap.

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Electron fractionalization under zero magnetic field

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Abstract

Electron fractionalization is of significant interest to both fundamental physics and topological quantum computing. The emergence of two-dimensional moiré materials provides a platform to explore the physics of electron fractionalization under zero magnetic field. In this talk, I will discuss two examples of zero-field electron fractionalization in moiré semiconductors: 1) the fractional Chern insulator that spontaneously breaks the time reversal symmetry, and 2) the time reversal symmetric fractional quantum spin Hall insulator.

Layered antiferromagnets under pressure

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Abstract

The rise of van der Waals materials opened up a new era in condensed matter and material science. After the discovery of graphene other materials including insulators, semiconductors, superconductors and topological materials have been found. The latest addition to this family was the discovery of 2D magnetic materials. These novel materials allow the development of novel spintronic devices including layered spin-valves or spin-orbit torque heterostructures.

In van der Waals heterostructures the coupling between layers often determines the behavior and the interaction strength. Pressure is a versatile tool allowing to tune the layer distance and hence the interaction strength. We have recently developed a novel system that allows the tuneability of these heterostructures without the need of special fabrication techniques [1]. We have shown that this allows to tune spin orbit strength in graphene-TMD structures [2-3], the topological properties of semimetals [4] or the band structure in twisted systems [5]. Similarly to these structures, the coupling between layers is a very sensitive knob in layered antiferromagnets.

In this talk I will show our recent measurements on layered antiferromagnets including CrSBr, which is one of the most promising candidates for spintronics applications and MnBi₂Te₄ which is claimed to be a Chern insulator. Our results show, that pressure not only allows to tune the magnetic properties, but as well as the topological properties.

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Many-body dynamics of magnons in chains of superconducting qubits

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Abstract

We explore how an Ising-type quantum phase transition manifests itself in a finite-size chain of superconducting qubits. In the paramagnetic phase, the chain supports magnon-like excitations, which are equivalent to collective electromagnetic excitations of the qubits. Local microwave spectroscopy allows measuring the spectrum of single-magnon as well as two-magnon excitations with a high frequency resolution. At a relatively small exchange coupling between the qubits, the single-magnon states are disconnected from the rest of the spectrum, and the low-energy dynamics is effectively a single-particle one. The magnon spectrum in this case is modelled well by a simple transverse-field Ising model. As the exchange coupling is increased, we observe evidence of coherent coupling of single-magnon and two-magnon excitations. As we increase the exchange coupling further the conversion dynamics becomes more complex. It involves nonnearest neighbor exchange couplings between the qubits, induced by common electromagnetic modes in the underlying qubit circuits. However, the spectrum contains signatures of the critical behavior, such as reduction of the energy gap and increased density of (multi-magnon) states. Our system realizes a new platform to simulate coherent many-body dynamics of magnetically ordered systems.

Solid state nanopores – fab to lab

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Apstract

To enable the use of solid state nanopores at the same scale as biological, imec has endeavored to manufacture the first sub-5 nm photolithographic pore in silicon nitride. To that end, imec is leveraging its lithography expertise to provide the first truly up scalable solid state nanopore platform which can be integrated with other silicon nanostructures. We have enabled lithographic nanopore fabrication using deep UV lithography in our 200 mm fab targeting a pore dimension of 20 nm, and are currently developing an extreme UV process in our 300 mm fab targeting sub-10 nm nanopores.

We aim to demonstrate that the imec lithographic nanopore provides a platform for future application work. To that end we developed a high throughput measurement platform allowing us to characterize hundreds of chips per day. Using data science we analyze thousands of nanopore chips to infer nanopore wettability, and its subsequent performance for translocation experiments. We show results of wafer to wafer variability in the 200 mm imec pilot line demonstrating a stable whole-wafer nanopore release process. We show our devices can provide DNA-scaffold based structure translocations comparable to standards in the field. Our next steps are enabling robust pore sensing over the span of a day, and en masse characterization of surface coatings and translocation experiments.

Ultralong 100 ns spin relaxation time in graphite at room temperature

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Abstract

Graphite has been intensively studied, yet its electron spins dynamics remains an unresolved problem even 70 years after the first experiments. Based on a detailed band structure calculation including spin-orbit coupling, an unexpected behavior of the relaxation times is predicted. We find, based on saturation ESR measurements, that T_1 is markedly different from T_2 . Spins injected with perpendicular polarization with respect to the graphene plane have an extraordinarily long lifetime of 100 ns at room temperature.

We provide a qualitative account of the observed spin relaxation based on the anisotropic spin admixture of the Bloch states in graphite obtained from density functional theory calculations. The extraordinary temperature dependence of the spin relaxation time and the *g*-factor are also elaborated. Moreover, insights into the granularity and undulations in graphene are considered, which translates into distribution of the local fields. Such findings are crucial for understanding mesoscopic transport measurements in (few layers of) graphene [1].



Figure 1. The spin-lattice relaxation time, T_1 , for the two orientations of the magnetic field (red triangles: B_{\parallel} , blue dots: B_{\perp}) in graphite as a function of temperature.

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Order parameter symmetries in BCS/BdG theory, and the Anderson prescription

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Abstract

Typically, a theorist asks the question of what particular symmetry a model interacti on will give rise to in the superconducting state by answering the question of which sy mmetry yields the highest critical temperature. This talk will explore generic tight-bindin g interactions and will illustrate that this methodology may be misguided; first the sym metry below the critical temperature (Tc) can deviate significantly from the one at Tc, a nd second, the behaviour of the order parameter near a surface can deviate significantly from the bulk.

Phonon signatures in the tunneling current through quantum dot-Majorana nanowire junctions

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Abstract

We propose a realistic nanodevice formed by embedding of a quantum dot between two conducting leads via symmetrical tunnel junctions in the presence of electron-phonon interaction. The quantum dot is coupled to one of the ends of a Majorana nanowire, which leads to probe Majorana bound states under conditions where the influence of an environmental bath, modeled here by a single long-wave optical phonon mode, on the tunneling current characteristics is considered. To analyze the transport characteristics of the nanojunction, a combination of the nonequilibrium Green's function technique with a canonical transformation has been employed. The corresponding retarded Green's functions have been determined by applying the equation of motion method. The behavior of the current vs. gate voltage, the current vs. bias voltage and the current vs. quantum dot-Majorana coupling characteristics is studied for an experimentally relevant parameter range. We demonstrate that the tunneling current is sensitive to, and depends non-trivially on the parameters of the dot-Majorana setup, in the regime of low voltages combined with low temperatures. The current-bias voltage curves present a step-like structure in the presence of electron-phonon coupling due to the phonon-assisted tunneling through the dot. We hope that our quantum dot-based setup can serve as a possible platform for future Majorana detection experiments.

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Reversible covalent bonds for transient tapping of single proteins in nanopores

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Abstract

This talk will present a strategy to trap single proteins inside nanopores for a duration that ranges from milliseconds to seconds. To this end, we coat solid-state nanopores with a protein-resistant polymer coating that is covalently functionalized with phenylboronic acid moieties (Fig. 1). The moieties can undergo the formation of reversible covalent bonds with vicinal diols on the carbohydrate moieties of glycated or glycosylated proteins. We demonstrate that the dwell time of trapped proteins can be controlled by the choice of pH of the recording electrolyte (Fig. 1) and by the magnitude of the applied potential difference across the nanopore. We take advantage of millisecond residence times to determine the shape and volume of single proteins with improved accuracy compared to freely translocating proteins. These experiments reveal that dwell times of at least 0.5 ms are needed to obtain the best possible accuracy in shape determination; residence times longer than this value provide only very small to no further benefit.



Figure 1. Concept of trapping single proteins with reversible covalent bonds. A) Solid-state nanopore with a protein-resistant polymer coating that exposes covalently attached phenylboronic acid moieties on its surface. B) Phenylboronic acid undergoes reversible covalent bond formation with vicinal diols on glycated proteins. Depending on the pH of the recording electrolyte and the applied voltage, these transient covalent bonds trap single glycated proteins for milliseconds to seconds making it possible to characterize the size and shape of these proteins.

Gating in Biological Nanopores

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Abstract

Biological nanopores are an emerging tool for the analysis and sequencing of a large range of molecules, from large biopolymers like DNA to small molecules such as metabolites. The working principle of biological nanopores relies on measuring the flux of ions through the biological nanopore under an applied voltage bias1. A limitation of nanopore sensing is gating behavior which is characterized by sudden, stochastic, and reversible drops in the pore ionic conductance unrelated to any analyte molecules. This effect pollutes the signal arising from translocation events. Although the gating phenomenon is omnipresent and undesirable, the underlying biophysical mechanism is unknown to this day. Here, we studied the gating behavior of single pore Aerolysin nanopores in D/C. Further we investigated the gating behavior of Aerolysin, a-Hemolysin and MspA nanopores through the memristive response of many-pore systems in A/C. These many pore experiments are high-throughput and allow for an easy assessment of the gating behavior of different pores. We find that gating depends on ionic strength, ionic species, temperature, and most drastically on the electrostatic potential in the pore lumen. Lastly, we discuss possible mechanisms for gating and their likelihood based on our data. Overall, these data provide a thorough quantification of gating behavior of multimeric beta-barrel forming nanopores, and strongly point towards a universal conformational change as the explanation of current reduction. Our work helps to increase the physical understanding of nanopore sensing which in turn could greatly improve biological nanopore sensors by reducing the likelihood of undesired gating effects. Further our findings can be used to rationally engineer desired electrical responses like those of diodes, providing the opportunity for the novel nanofluidics circuitry. This is particularly challenging at this length scale for any other nanofluidics system.

From Solid-State to Biophysics XI Dubrovnik (Croatia), 8-15 June 2024



Figure 1. A Aerolysin cross section through the lumen with positive and negative amino acids labelled and the electrostatic potential of aerolysin wild type (green), K238AK242A (yellow), D216A (turquoise), K238A (grey) calculated from all atom simulations at +200 mV and -200 mV. Gating behavior measured with different aerolysin mutants in AC (0.1 Hz, 200 mV amplitude sinusoidal) B Gating behavior of aerolysin wild type with its positively charged lower lumen, the pores gate at negative applied voltages. C K238A K242A, a mutant with a negatively charged lower lumen, the pores gate at positive voltages. D Mutant D216 with a positively charged upper and lower lumen which exhibits gating both at positive and negative voltages. E K238A a largely uncharged mutant which shows no gating at this applied AC voltage. Each plot displays the open pore IV curve in black and a representative charge distribution of the lumen of the respective mutant.

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Electro-optical sensing of single protein biomarkers in nanopores and nanochannels: towards digital proteomics

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Abstract

Nanopores are single molecule biosensors that utilize electrokinetic forces to focus, linearize and detect individual biopolymers, such as DNA and proteins.¹ Solid-state nanopores are mechanically robust, versatile sensors, that lend themselves for integration in sophisticated devices designed to processes and detect biological samples. Our lab is pursuing this technology to advance wide range of biomedical needs. Here I will provide several recent examples, including: (i) Threading and imaging of an extremely long genomic DNA (~0.5 Mbp) into solid-state nanopores and engineering the Electro Osmotic Forces (EOF) to facilitate the sensing of extremely short DNA (<50 bp) in sub 5 nm pores. (ii) An amplification-free mRNA quantification sensors to replace RT-qPCR for SARS-CoV-2 and for quantification of the early-stage Colorectal cancer marker MACC1. Moving beyond nucleic acids, I will discuss our latest efforts towards the use of electrophoretic single protein molecule separation by mass/charge ratio in sub-wavelength, nanometric channels.^{2,3} Two color sensing and dynamical tracking of dually labelled proteins enable proteins identification using 4D information. This antibody-free sensing methodology permits discrete quantification of a cytokine panel, for the discrimination among viral versus bacterial infections host's response. Moreover, we show that this method allows identification of close VEGF protein *isoforms*, with diverse biological role, but can evade immuno sensing. This method can be integrated upstream of the many other single molecule methods including nanopore sensors and fluorosequencing for enhanced, high-throughput proteome profiling.

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Controlled sensing of user defined aptamer-based targets using Scanning Ionic Conductance spectroscopy

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Abstract

Solid state nanopores offer strong possibility for the detection of disease biomarkers for early diagnostics applications. Standard approaches harness finger-typing approaches where protein targets are bound to DNA carriers and detected in free translocation with a solid state nanopore. However, they suffer from several drawbacks including uncontrolled fast translocations, which leads to low detection accuracy and high false negative. Here, we propose a nanopore based system capable of sensing selected molecules of interest from the biological fluids by harnessing programmable aptamers sequences attached on DNA carrier systems that are tethered on glass surfaces. This allows for spatial and velocity control over translocation and repeated scanning of the same analyte. We demonstrate repeated scanning of the same aptamer target site of >5 times. Our approach allows for a detection accuracy of up to 50%, significantly more than the $\sim 10\%$ when compared with standard solid state nanopore approaches. Additionally, the strong spatial control allows for significantly increased densities of aptamer target sites along the same DNA carrier, thereby paving the way for multiplex sensing. Our system also allows for user-defined programmability with different aptamer sequences expanding the use of our system for sensing of other disease biomarkers.



Figure 1. Design concept for using DNA aptamers and a carrier for protein sensing.

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Probing Dynamic Structural Changes in Nanocatalysts during Reaction with In Situ TEM

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Abstract

Nanoparticle catalysts are commonly used to accelerate chemical reactions and increase the efficiency of a broad range of industrially relevant reactions. To enable the rational design of catalysts with better performance, it is critical that we understand the relationship between a nanoparticle's structure and its catalytic properties. However, because the nanocatalysts exhibit active structures only during the reaction, insights about how catalysts work must be obtained under relevant reaction conditions. Recent developments in in situ environmental TEM, now allow us to study nanostructures within a liquid or gas environment with TEM, and probe their dynamics in operando.

Here, using in situ gas-phase TEM imaging, I will discuss how nanoparticle catalysts behave during catalysis and identify transient active states responsible for reactions. Specifically, using monometallic and bimetallic nanoparticles for the CO oxidation model reaction, I will describe surprising permanent and transient structural transformations that drive the CO-oxidation reaction.

These insights into how nanoparticle catalysts evolve during during catalysis are important for the rational design of high-performance catalysts.

Magnetic behaviour of chain and layered hybrid methoxyethylammonium halocuprates(II)

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Abstract

Increasing number of studies in recent times suggest that layered hybrid organic-inorganic halometallates pave the way for unveiling the intricacies of quasi-two-dimensional systems, which hold both fundamental and applicative value.[1] Novel studied hybrid compounds of methoxyethylammonium halocuprates(II) crystallize either in a chain or layered structure. Here, we examine the magnetic behaviour of several such structures over a wide range of temperatures and magnetic fields using the SQUID magnetometer. By modeling static magnetization, we determine the strength of magnetic interactions and describe the dimensionality of the magnetic subsystem, widening the understanding of the fundamental mechanisms of magnetic phenomena and the development of new materials and methods aimed at optimizing their properties.[2][3] Methoxyethylammonium chlorocuprate(II) compounds with chain topology behave as ferromagnetic spin chains, while those with sheet topology display ferromagnetic transition around 6.4 K and relatively soft ferromagnetic behaviour. Measuring plate-like crystals of the same layered material, easy magnetic plane and hard magnetic axis were observed. On the other hand, methoxyethylammonium bromocuprate(II) compounds with chain topology display broad maximum of magnetization around 90 K, which is characteristic of antiferromagnetic spin chains with relatively stronger super-exchange interaction.

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Peptide Microdroplets with Tunable Biophysical Properties for Programmable Intracellular Delivery of Macromolecules

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Abstract

Biomacromolecular therapeutics (*e.g.*, proteins, DNA, mRNA, antibodies, gene editing tools, etc...) hold vast therapeutic potential across human disease states by addressing intracellular targets that have proven refractory to traditional approaches. However, a common hurdle to the deployment of these modalities lays in their inability to cross the cell membrane, which has prompted intense research into the development of safe delivery vehicles capable of packaging large biomacromolecules and deliver them intracellularly. A promising type of delivery vectors that we have recently pioneered are phase-separating peptide (PSP) coacervate microdroplets (CMs) produced by liquid-liquid phase separation (LLPS)^{1,2}. CMs are simple to synthesize, non-cytotoxic, and can recruit a wide range of modalities (proteins, pDNA, mRNA, gene editing tools ³, etc...) using aqueous-phase preparation procedures. While we have demonstrated that PSP CMs are able to cross the plasma membrane of mammalian cells and deliver their payload, the properties of CMs that regulate their cell uptake and cargo release kinetics remains poorly understood.

In this talk, I will present our recent studies showing that cell uptake and cargo release kinetics efficacy can be modulated by controlling the materials and biophysical characteristics of CMs, which can be achieved by simple mutations of PSPs. I will then discuss how optimized PSP sequences can yield remarkable delivery efficacy of a broad range of therapeutics, including proteins, antibodies, genes, mRNA, siRNA, and CRISPR-Cas9 modalities, all of which can be transfected into cells with an efficacy that surpass currently available commercial delivery systems, including in hard-to-transfect cells such as primary cells, immune cells, and macrophages.

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On the way to full and exact control of the nonlinear electron-phonon coupling

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Abstract

I present a numerically exact study of polaron with quadratic electron-phonon coupling (proportional to the square of displacement $\sim x^2$), or X2 polaron, using two alternative methodological developments [1,2]: Diagrammatic Monte Carlo (DMC) and X-propagators (X-P) techniques. The results cover both antiadiabatic and adiabatic regimes and the entire range of electron-phonon coupling g_2 , from the system's stability threshold at attractive $g_2 = -1$ to arbitrary strong repulsion at $g_2 >> 1$. The key properties of X2 polarons prove dramatically different from their linear counterparts. They (i) are insensitive even to large quadratic coupling except in the antiadiabatic limit near the threshold of instability at attraction, (ii) depend only on the adiabatic ratio but are insensitive to the electron dispersion and dimension of space, and (iii) feature weak lattice deformations even at the instability point. Our results are directly related to the properties of electrons at low densities in polar materials [3], including recent proposals for their superconducting states.

I show how the X-P technique can be generalized to any kind of nonlinearity $(\pm \alpha x^2 \pm \beta x^4)$, Jahn-Teller and Pseudo-Jahn-Teller type, and even that obtained in ab-initio band structure calculations) and to any dispersion of phonon branch leading, thus to full and exact control of the anharmonic electron-phonon coupling.

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Multi-material additive manufacturing of metals at the nanoscale: an electrochemical approach

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Abstract

Additive manufacturing, also commonly known as 3D printing, is rapidly becoming a part of our everyday life: from DIY use by hobbyists to industrial production, 3D printing is experiencing a booming success. The technologies advance quickly with faster print rates, broader choice of materials and a constantly increasing accuracy and printing resolution. Impressively, state-of-the-art techniques take the printed feature sizes to the extreme: multiphoton optical stereolithography and focused electron or ion beams are now capable to produce objects with nanoscale resolution. Although at the cutting edge to printing finest details, these advanced manufacturing methods lack the capacity to process dense and pure electrical conductors – materials very much needed to push the limits of the technologies of the future – sensors, energy storage devices, logic gates and memory interfaces.

Electrochemical methods, which have an advantage to process a wider range of materials – conductors and semiconductors, bulk materials and colloids, at a first glance, have little to do with additive manufacturing. Electrodeposition, a well-established approach traditionally used to produce metallic coatings or thin films, is often integrated in microfabrication process but is limited to planar two-dimensional designs. However, when combined with state-of-the-art nanoelectrochemical approaches, electrodeposition can be taken into a three-dimensional realm, where it can be used to produce complex structures with micro- and nanoscale dimensions [1]. The key to achieve this is nanoscale confinement combined with layer-by-layer additive processing. Liquid manipulation by pressure driven flow through nanoscale cantilevers [2] or intermittent meniscus formation using nanodroplets [3] – a variety of nanoelectrochemical and physicochemical challenges to overcome. Here, strategies to achieve multi-material 3D nanofabrication of intricate metallic structures are presented.

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Supramolecular Chiral Systems Induced by Mechanical Manipulation: Utilizing Pyrazinacene-Based Chiral Assemblies

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Abstract

The fabrication of chiral assemblies from initially achiral molecules has received significant attention due to its implications for understanding biological structures and self-assembly processes, ^[1,2] particularly in the realm of supramolecular chirality. In this study, a dynamic interfacial assembly strategy is employed to generate unique chiral assemblies from achiral pyrazinacenes^[3] which are linear nitrogen-rich acene derivatives. These assemblies manifest as one-dimensional supramolecular J-aggregate tapes, which, intriguingly, coils into Archimedean spirals of uniform width. Furthermore, the dynamic nature of the assembly process allows for the controlled transformation of these Archimedean spirals into tightly coiled toroids and chiral concentric vortices. Analysis via synchrotron -based grazing incidence X-ray diffraction shows a lamellar columnar oblique mesophase-like structure in the J-aggregate monolayer formed through the layer-by-layer deposition technique. The ability to generate chiral supramolecular assemblies from achiral supramolecular assemblies and proximity-coupled material applications.



Optional Figure 1. Self-assembling Pyrazinacens for Archimedean Spirals.

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Photovolatic effects below the electronic band gap

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Abstract

In solid state physics, the notion of geometry and topology for Bloch electrons in solids has provided a new insight into the light-matter interaction in this decade. One such example is the bulk photovoltaic effect called "shift current" that arises from a geometrical (Berry) phase of a Bloch wave function and has a close relationship to the modern theory of electric polarization [1]. While most previous studies of the bulk photovoltaic effects have focused on the photocurrent due to the above band gap excitations of noninteracting electrons, systems of correlated electrons have a potential to support a novel nonlinear functionality. In this talk, I will present novel nonlinear optical effects originating from unique excitations in correlated electron systems, especially those below the electronic band gap that are enabled by shift current mechanism along with electron interactions, including excitons in semiconductors [2], magnetic excitations in multiferroic materials [3], and phonon excitations in electron-phonon coupled systems [4].

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Theory of Anomalous Crystal Shapes of Various Topological Insulators

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Abstract

A topological crystalline insulator (TCI) is a topological phase characterized by crystallographic symmetries. There exist various TCI phases depending on the crystallographic symmetries, such as mirror- symmetric TCIs and glide-symmetric TCIs [1,2]. In these TCIs, whether or not gapless topological surface states appear depends on the surface orientations. Namely, if the surface orientation is mirror/glide invariant, the corresponding gapless surface states appear depends on the parity of the Miller index of the surface.

In this presentation, we discuss relationships between equilibrium crystal shapes and topological phases. When gapless topological surface states appear, the surface energy for the surface orientation will become higher. It makes this surface orientation less favorable, and its area will become smaller. Therefore, we expect that the equilibrium crystal shape will depend on whether the crystal is in a trivial phase or in a topological phase. By model calculation, we show that this is indeed true for various topological phases [3,4]. If time allows, we will introduce our ongoing work on theory of crystal growth of topological insulators.



Figure 1. Calculated equilibrium crystal shapes for (a) a trivial insulator and (b) a TCI.

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Murunskite: Metallisation by chemical doping

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Abstract

Mastering the growth of high-quality murunskite ($K_2FeCu_3S_4$) monocrystals, we have achieved a significant breakthrough in the research of a new material with interesting magnetic and electric properties. The parent compound of murunskite shows semiconducting behaviour with an antiferromagnetic transition at 100 K, with resistivity and optical conductivity measurements showing characteristics similar to cuprate parent compounds. In contrast to electronic properties being more similar to cuprates, murunskite is isostructural to the 122 family of ferro-pnictides. Accordingly, murunskites can be described as a bridge between cuprates and ferro-pnictides, the best known high-temperature superconductive materials at atmospheric pressure [1].

Furthermore, DFT calculations show that the sulfur 3p orbitals of the parent compound are partially open, making them accessible for charge manipulation. Finally, the possibility of tuning the bond polarity and orbital occupation, with the goal of manipulating the balance between localization and delocalization of electrons - ie. between ionicity and metallicity, holds promise for understanding the appearance of superconductivity in ionically bound materials in general.

With this in mind, we have started developing substitution strategies on both, ligand sites with As and Se, and metal sites with Zn, Co, and Ni. The novel synthesized single crystals are carefully characterised by a wide range of experimental methods such as magnetic and resistivity measurements, energy dispersive x-ray and x-ray diffraction.

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Investigating material properties of Dhh1-RNA condensates using optical tweezers

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Abstract

Dhh1 is an important highly conserved Deadbox RNA helicase protein that regulate mRNA processing in the cell through the formation of biomolecular condensate which acts as processing bodies. However, their material properties which affect their biological function to sequester, process and release mRNA such as fluidity and viscosity are not well understood. Here we use optical tweezers and active microrheology assays to elucidate the material properties of dhh1 droplets. First, through controlled fusion of droplets with our dual beam optical tweezers, the fusion time of the two droplets informs on the ratio between the inner viscosity and interfacial tension. Here we show that the droplets became more liquid like on increasing pH and salt concentration. We also found evidence for hydrotropic effect of ATP on Dhh1-PolyU condensates. Our results suggest that, ATP hydrolysis prevented LLPS at higher pH while the condensates became more gel-like at lower pH on ATP hydrolysis. These results inform us on various biochemical mechanisms that cells might employ to control properties of biomolecular condensates. Second through the use of microrheology assays where beads are embedded inside the droplets and made to oscillate with optical tweezers, we are able to obtain the viscoelastic moduli and the interfacial tension of the condensates. We explore the role of parameters such as pH, salt concentration, temperature and ATP on the viscoelasticity of the condensates. Our results lead to further our understanding of Dhh1 and the role they play in intracellular function.
EuCd₂X₂: Semimetal illusion versus Semiconductor reality

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Abstract

The search for intrinsic magnetic topological materials has captured the interest of numerous scientists in recent years due to their potential spintronic application. EuCd2X2 (X = Sb, As, P) family was predicted by Density Functional Theory (DFT) to be a topological, Weyl semimental [1-2]. This claim was further supported by transport measurements and Angle-Resolved Photoemission Spectroscopy (ARPES), which exhibited metallic-like resistivity and the conical shape of the valence band, respectively [3-4].

However, our recent infrared- and magneto-optics measurements revealed that $EuCd_2X_2$ is a magnetic semiconductor rather than a topological Weyl semimetal. We obtained energy gaps of 0.5 eV, 0.77 eV, and 1.2 eV for X = Sb, As, and P, respectively [5] [6]. These band gaps are notably influenced by the application of a magnetic field, undergoing redshifts of 45 meV, 125 meV, and 150 meV, respectively. Despite these shifts, magneto-optics shows that the band gaps do not close even under the application of a high field of 35T, indicating that the compounds remain semiconductors and thus excluding a magnetic Weyl semimetal scenario.

Additionally, ARPES and pump-probe ARPES on EuCd₂As₂ confirmed the band gap of 0.7 eV. The resistivity measurements revealed activation behavior for EuCd₂As₂ and EuCd₂P₂, while EuCd₂Sb₂ exhibited metallic-like resistivity, implying that the system is doped.

In conclusion, our study provides valuable insights into the effects of element substitution on the electronic band structure of EuCd2X2 semiconductors.

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Molecular Switches with Changing Switching Probabilities for Emulating Synaptic Behavior

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Abstract

Our brains constitute a molecular computer that is able to process enormous amounts of information with a tiny energy budget [1]. Inspired by the energy efficiency of brains and the ever-increasing demand for miniaturised electronics, there is a drive to develop devices that mimic the dynamic character of neurons and synapses. To achieve this goal, brain-like computing is emulated with energy inefficient and complex silicon-based circuits or with mesoscale memristors, but these approaches still require large amounts of energy. For these reasons, it is important to develop new types of hardware that can mimic brain-like computation processes [1,2]. We have been developing molecular switches that behave like synapses with the aim to realize spiking neural networks. I will introduce a new type of molecular switch that can remember its switching history [3]. By coupling fast electron transport to slow proton addition steps via dynamic covalent bonds, the switches display time-dependent switching probabilities which can be used for brains-inspired and reconfigurable electronics [4,5]. These artificial synapses are promising to develop alternative neural networks and open new ways to design electronic devices by exploiting their inherent dynamical properties.

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Anomalous Hall signal in insulating EuCd₂As₂

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Abstract

 $EuCd_2As_2$, an A-type antiferromagnet with a transition temperature of 9.5 K, has recently garnered significant interest in the community dealing with topological semimetals. Initially, it was reported to be an ideal Weyl semimetal, but it was later identified as a magnetic semiconductor with a gap of approximately 0.8 eV [1]. Despite this apparent downgrade in material properties, $EuCd_2As_2$ exhibits numerous intriguing physical properties. These include colossal magnetoresistance, a natural spin-valve structure, a low-field transition to a forced ferromagnetic phase at around 1.5 T, and the ability to tune the Fermi energy position.

In our presentation, we will focus on the anomalous contribution to the Hall signal observed in the paramagnetic phase of insulating samples, which is not observed in metallic samples. This effect has been associated with an extrinsic phenomenon involving the formation of spin clusters, similar to recent observations in EuAs [2].

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Materials for the future

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Quantum hybrids of superconductivity and magnetism via topological solitons

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Abstract

Topological solitons and quantum mechanics have been intertwined for the past sixty years. Even before the term soliton had been coined, Abrikosov's theory predicted the formation of vortices in the phase field of superconductors, an exemplar exposition of macroscopic quantum coherence. Recent work shows that solitons are in fact a timely and promising platform for quantum operations. I will demonstrate the viability of using spin topology to influence a superconductor at selective length scales through a completely new material architecture namely, a stack of magnets and a superconductor that shows stable vortices above elongated chiral spin textures, as well as isolated skyrmions. This is an excellent geometry for fluxonics and chiral superconductivity, as well as quantum processes such as non-perturbative, non-contact Majorana braiding.

Selective Mass Permeation Property of Low-Dimensional Materials

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Abstract

Selective mass transport inside, across, and between nanoscale low-dimensional materials such as nanotube, graphene, and molybdenum disulfide, respectively, forms the basis of the low-dimensional nanofluidic phenomena and poses various potential engineering applications. This talk will briefly review an existing paradigm of fast transport in carbon nanotube conduits with a proposal of a new scaling relation to answer the question, "How fast is fast?" Then follows our story of shifting the paradigm with recognition of equivalence between a nearly frictionless channel and no-channel-but-only openings. Synthesis, transfer, perforation, and device integration of graphene enable altogether preparation of an atomically thin, porous membrane for the embodiment of this new concept. Transport physics across the orifice points to an ultimate permeation of fluids (both in molecular and viscous transport regimes), heralding a high-flux membrane.

On the other side of the selectivity-permeance spectrum lie molecular conduits such as nanopores and slits formed in and between two-dimensional materials. In this regard, this talk reports our understanding of the ion-selective transport mechanism in nanopores as well as the realization of "waterene," *viz* monolayer of water, in between molybdenum disulfides. Metrology, dynamics, and hydration of waterene will be discussed.

Cryo-electron microscopy with a laser phase plate

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Abstract

Cryo-electron microscopy can visualize biomolecules at high resolution in a near-native state, but the technique is limited by the low contrast of specimens together with their sensitivity to electron radiation. To maximize image contrast, a phase plate can be employed to apply an additional delay between the scattered and unscattered beams in a diffraction plane of the microscope. While this approach is widely used in optical microscopy, phase plates developed for electron microscopy have been prone to being charged by or scattering the electron beam, leading to unstable behavior and resolution loss.

To overcome these limitations, we have developed a laser-based phase plate (LPP). A laser beam, amplified and focused by a Fabry-Perot optical cavity, intersects the unscattered electron beam to impart the desired phase shift. The LPP provides a stable phase shift over hours while keeping material objects far from the electron beam path to avoid scattering and decoherence.

The reliability of the LPP paves the way for several future directions in cryo-electron microscopy and tomography. Improved contrast at low spatial frequencies enables detection of small particles inaccessible to conventional (defocus-based) phase contrast imaging, as well as superior correction of beam-induced motions. Additionally, the LPP eliminates the need for specimen defocus and, in combination with a spherical aberration corrector, permits near-perfect contrast transfer over many orders of magnitude in resolution (from ~100 nm to 0.1 nm). Simultaneous visualization of both small and large structural features promises to benefit cryo-electron tomography by providing high-resolution information together with larger-scale context.

I will show our progress on single-particle reconstructions and tomography with the LPP and discuss prospects for the new imaging modalities enabled by the LPP based on a combination of experiments and simulations.

Quantifying Immune Cell Dynamics: Establishing a Novel Large Field of View Light Sheet Microscopy Platform to Study Cellular Function across Space and Time

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Abstract

The physics of immune cells is increasingly considered as a primary determinant of their function and behavior. T cells, key players of the human adaptive immune response, exhibit considerable diversity in their behavior and function even at the single-cell level. Emerging evidence suggests that comprehending immune cell function necessitates not only understanding the omics and biochemical pathways, but that it is also the spatiotemporal context that shapes immune cell function and behavior. Quantifying the dynamic interplay of physical and biological features has therefore become an important challenge in the biomedical sciences. To address this key problem, we have developed a novel minimally invasive light sheet-based microscopy platform. Our platform leverages an ultra-thin super-extended (UTSE) light sheet and a machine learning-based automated data analysis pipeline. This cutting-edge microscopy technique offers a large field of view of 5 mm enabling the simultaneous quantification of signaling events from up to 100,000 cells over periods ranging from a few seconds to multiple days. By applying the UTSE technology to relevant biological cytotoxicity assays, we aim to elucidate the correlation between early calcium activation signaling, immunological synapse formation, and T cell effector function. This technology unlocks the potential to enhance microscopy's sensitivity to rare biological events, enabling the identification of rare behavioral cell subpopulations that may drive and underlie health and disease.

Electronic structure modulations induced by intercalation of magnetic 3d ions into 2H-NbS₂

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Abstract

Layered compounds, because of their reduced dimensionality, are prone to different instabilities that can lead to various, sometimes exotic, electronic phases. Their layered structure allows for exfoliation and often intercalation, making them promising candidates for new electronic devices and applications. Transition-metal dichalcogenides (TMDs) are prominent members in this class of compounds featuring various charge density waves, metallic and semi metallic, superconducting and Mott insulating states. Intercalation with transition metal ions introduces magnetic sublayers leading to intricate coupling between metallic and magnetic degrees of freedom. Co1/3NbS2 and Ni1/3NbS2 both exhibit antiferromagnetic ordering below their respective Néel temperatures, $T_{N,Co} = 28$ K and $T_{N,Ni} = 95$ K. However, while magnetic order in $Co_{1/3}NbS_2$ is completely suppressed under moderate pressure ($p_c = 1.7$ GPa), $Ni_{1/3}NbS_2$ shows enhanced magnetic ordering in this pressure range. The electronic transport anisotropy further highlights the different roles that Co and Ni play upon intercalation. This difference is also evident in the electronic structure of the two compounds, investigated here using angle-resolved photoemission spectroscopy (ARPES), ab initio electronic structure calculations, and modeling. It is shown that intercalated ions dominate the interlayer coupling. In $Co_{1/3}NbS_2$, we propose a "spin-valve" mechanism where the intercalated Co ions act as spin-selective electrical transport bridges between host layers. Conversely, in Ni1/3NbS2, the Ni ions' orbitals effectively suppress electrical connections between layers.

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Nonequilibrium transport and thermalization in two-dimensional bad conductors

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Abstract

One of the most fundamental questions in physics is whether an isolated quantum manybody system thermalizes a long time after it is prepared far out of equilibrium. Recently, there has been a lot of interest in mechanisms that break ergodicity and lead to the absence of thermalization. In strongly disordered quantum systems, many-body localization (MBL) provides a robust mechanism for the failure of thermalization, but many questions remain open, especially in dimensions D > 1. At the same time, experiments have been limited to those on synthetic quantum matter, such as ultracold atoms in optical lattices and superconducting qubits, while observing the absence of thermalization in real, solid-state materials has been a challenge.

This talk will describe the experimental studies of nonequilibrium dynamics in strongly disordered D=2 electron systems realized in Si heterostructures and weakly coupled to a thermal bath. Charge dynamics is studied using time-resolved conductivity measurements following a quantum quench protocol, in which the electric field-effect is employed to change the electron density instantaneously. Furthermore, measurements are performed for different densities across the quantum metal-insulator transition. We consider the case of power-law interactions $\propto 1/r^{\alpha}$, with α =1 and α =3. We find that, for α =1, the system thermalizes, although the dynamics is glassy. The behavior of this Coulomb glass is similar to that of a large class of both 3D and 2D systems that are out of equilibrium (e.g., spin glasses, supercooled liquids). In contrast, in the case of a screened or dipolar Coulomb interaction (α =3), the thermalization is anomalously slow and strongly sensitive to coupling to the thermal bath, consistent with the proximity to a MBL phase. In both cases, slow dynamics is observed only when $k_Fl < 1$ (l – mean free path, k_F – Fermi wave vector), i.e. for strong enough disorder when the 2D electron system becomes a bad conductor.

This direct observation of the MBL-like, prethermal regime in an electronic system clarifies the effects of the interaction range on the fate of glassy dynamics and MBL in 2D. These are important insights for theory, especially since the results have been obtained on systems that are much closer to a thermodynamic limit than synthetic quantum systems employed in previous studies of MBL. By establishing a new, versatile solid-state platform for studies of thermalization and MBL in large systems, our work also opens new possibilities for further studies of ergodicity breaking and quantum entanglement in real materials.

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Broken symmetries and tissue dynamics

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Abstract

Using generalized hydrodynamic theory, I will describe how a nematic epithelium can be totally at rest on a narrow stripe and spontaneously adopt a shearing motion due to cell contractility on broader stripes. Such shearing motions are observed in cancer invasion. I will then describe experiments in which the substrate plays the role of an external orientational field on the nematic direction of the tissue. The simple case of a homogeneous field meant to mimic extracellular matrix is for some cell lines spectacular: a new symmetry breaking toward a polar moving state is observed. Again, generalized hydrodynamics allows to understand this polar symmetry breaking. I will then show that substrate curvature may play the role of external field and illustrate this statement with experiments investigating epithelium motion in hollow cylinders or on cylindrical fibers. Spontaneous symmetry breaking is again observed, with a continuous rotation of the tissue orthogonally to the cylinder axis. In this case the motion is due to cryptic lamellipodia. I will eventually argue that the physical approach to tissue dynamics is relevant to real life situations.

AI for Multi-Omics Data Fusion to Enable Precision Medicine

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Abstract

Large quantities of heterogeneous, interconnected, systems-level, molecular (multi-omic) data are increasingly becoming available. They provide complementary information about cells, tissues and diseases. We need to utilize them to better stratify patients into risk groups, discover new biomarkers and targets, re-purpose known and discover new drugs to personalize medical treatment. This is nontrivial, because of computational intractability of many underlying problems on large interconnected data (networks, or graphs), necessitating the development of new algorithms for finding approximate solutions (heuristics) [1].

We develop a versatile data fusion artificial intelligence (AI) framework, that also utilizes the state-of-the-art network science methods, to address key challenges in precision medicine from the multi-omics data: better stratification of patients, prediction of biomarkers and targets, and re-purposing of approved drugs to particular patient groups, applied to different types of cancer [2,3], Covid-19 [4,5], Parkinson's [6] and other diseases. Our new methods stem from graph-regularized non-negative matrix tri-factorization (NMTF), a machine learning technique for dimensionality reduction, inference and co-clustering of heterogeneous datasets, coupled with novel network science algorithms. We utilize our new frameworks to develop methodologies for improving the understanding the molecular organization and diseases from the omics data embedding spaces [7,8,9].

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The potential roles of autophagy in auditory neuron morphology during stimulation with pulsed electro-magnetic fields and in guided neuron growth using microtopographical cues

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Abstract

Spiral ganglion neuron (SGN) health and regeneration have gained significant research interest due to their crucial role in cochlear implantation's success in treating hearing loss. One of the main predictors of its success is the number of surviving SGNs and their proximity to the cochlear implant electrodes. Here, we examine autophagy, a genetically conserved self-degradation pathway that removes damaged cellular components and supports cellular homeostasis, as a potential target for modulating neuronal viability and morphology. Research shows that autophagy activation protects SGN health in the face of ototoxic factors [1] and is also involved in neuronal development [2]. Specifically, it was shown that the effects of electromagnetic stimulation and microtopographical cues have been linked with the mammalian target of rapamycin (mTOR) pathway, the master regulator of autophagy [3]. However, it is unknown whether mTOR signaling has a role in neonatal SGN growth during electromagnetic field (EMF) stimulation undergoing microtopographical-based mechanotaxis. We propose an experimental design that aims to shed light on this relationship and thus potentially enhance therapeutic strategies for patients with sensorineural hearing loss.

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Universal thermodynamics of the planar Bose gas: Functional Renormalization Group vs experiments

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Abstract

The Functional Renormalization Group (FRG) is a powerful field theoretic method to tackle strongly correlated systems, allowing for describing both universal and non-universal properties. We will review recent results obtained with this method to describe ultracold atom experiments, focusing on the case of planar Bose gases, i.e. cold gases confined in a plane. In particular, we will demonstrate that simple approximations of the FRG flow equation allows for describing the thermodynamics of the such system, which is particularly challenging due to strong phase fluctuations and the associated Kosterlitz-Thouless physics. We find a very good agreement with experimental results.

Murunskite: a bridge between cuprates and pnictides

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Abstract

Despite exceptional scientific efforts over several decades, there is almost no universal agreement about the superconducting state of cuprate compounds. A constructive wa to improve understanding would be to synthesize and investigate a new system, which displays superior chemical flexibility and tunability of the valence of the transition metal ions. One could then manipulate its various electronic, metallic, and mechanical properties. We study murunskite, which interpolates between cuprates and pnictides[1]. This presentation will report the successful growth and characterisation of the first-ever high-quality Murunskite single crystals. These crystals show semiconductors like the parent compounds of cuprates, yet isostructural to the metallic iron-pnictides. Moreover, like both families, it has an antiferromagnetic response with an ordered phase below 100 K.Spectroscopy (XPS) and Density Functional Theory (DFT) calculations concur that the sulfur 3*p* orbitals are partially open, making them accessible for charge manipulation, which is a prerequisite for superconductivity in analogous layered structures. Furthermore, DFT indicates that the valence band is more cuprate-like, while the conduction band is more pnictide-like. We also managed to substitute Fe with Co in the parent compound, leading to superconductivity in this family for the first time.



Comparison of murunskite structure b) with a cuprate a) and pnictide c)

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Characterizing proximity induced spin-orbit coupling in graphene by quasiparticle interference imaging

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Abstract

Inducing and controlling spin-orbit coupling (SOC) in graphene is key to create topological states of matter, and for the realization of spintronic devices. The most successful strategy to achieve this goal so far is to place graphene onto a transition metal dichalcogenide. However, there is no consensus as to the nature and the magnitude of the induced SOC. In this talk, we show that the presence of backscattering in graphene-on-WSe2 heterostructures can be used to probe SOC and to determine its strength quantitatively, by quasiparticle interference (QPI) imaging using a scanning tunneling microscope. Analyzing QPI images of heterostructures with selected twist angles between 0° and 30°, we find that the induced SOC consists of a valley-Zeeman ($\lambda vZ \approx 2 \text{ meV}$) and a Rashba ($\lambda R \approx 15 \text{ meV}$) term. These results are in excellent agreement with transport experiments, both finding that the Rashba term is an order of magnitude larger than current theoretical predictions. QPI further gives unambiguous evidence that the measured SOC is the result of a modified band structure and demonstrate a viable strategy to determine SOC quantitatively by imaging quasiparticle interference.

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Aqueous Nanoscale Systems

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Abstract

Water is the most important liquid for life. It is intimately linked to our well-being. Without water, cell membranes cannot function. Charges and charged groups cannot be dissolved, self-assembly cannot occur, and proteins cannot fold. Apart from the intimate link with life, water also shapes the earth and our climate. Our landscape is formed by slow eroding/dissolving processes of rocks in river and sea water; aerosols and rain drops provide a means of transport of water. Because of the complexity of liquid water and aqueous interfaces, the relationship between the unique properties of water and its molecular structure has not been solved.

Techniques that can provide femtosecond structural information over multiple length scales can help. For this purpose, we developed nonlinear light scattering [1] and imaging tools [2] to access molecular structural information of aqueous solutions and interfaces. With our new approaches we have found nanoscale ordering in dilute salt solutions [3], and probed the structure of aqueous nanoscale interfaces relevant for chemistry and biology: emulsions [4], lipid droplets [5], liposomes [6], water droplets [7] and oxides [8]. We solved the mysteries behind the Jones-Ray effect [3] and the origin of charge on neutral oil droplets in water, which underlies hydrophobicity [9]. The optical properties of water can also be used to determine the electrical potential (voltage) of interfaces. This unique spatiotemporally resolved hydration readout is useful for obtaining new insights relevant for chemistry [2], biophysics [10], neurology [11] and catalysis [12]. This presentation will highlight some of our recent findings.

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Single-molecule lifetime imaging with a gated single-photon camera

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Abstract

Fluorescence lifetime imaging microscopy (FLIM) is a powerful tool to discriminate fluorescent molecules or probe their nanoscale environment. FLIM is used in particular for molecule discrimination in the recently reported first demonstration of a single-protein sequencer¹. FLIM is commonly realized through time-correlated single-photon counting (TCSPC), which is precise but intrinsically low-throughput as it normally probes one molecule at a time². Time-gated cameras have been shown to enable high-throughput FLIM on bright samples with dense labels², but their application to single-molecule microscopy has remained underexplored.

Here, we report fast and accurate single-molecule FLIM with a commercial time-gated single-photon camera. We identify the optimal acquisition scheme that results in single-molecule lifetime measurements only ~2-3 times less precise than TCSPC with a given photon count, while enabling multiplexing over thousands of molecules simultaneously (Figure 1). This allows us to bring the time needed to screen the lifetimes of a population of molecules on a surface from the timescale of a day to the timescale of a minute (Figure 2). We apply this approach to the imaging of aerolysin pore-forming toxins in supported lipid bilayers, and explore their assembly from labeled monomers through lifetime-based single-molecule Förster resonance energy transfer (smFRET)³. Finally, we show that our imaging scheme can enrich wide-field single-molecule localization microscopy techniques such as STORM and PAINT with lifetime information, opening new routes towards super-resolved multi-target imaging and environment sensing³.



Figure 1. Setup and acquisition scheme for high-throughput single-molecule fluorescence lifetime imaging.

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Figure 2. Wide-field fluorescence lifetime imaging of aerolysin pore-forming proteins labeled with Cy3B fluorophore. 1 minute of measurements yields >300 molecules, which is enough to build the lifetime histograms presented. The standard approach of confocal imaging would take a full day of active measurements to get to the same result.

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Learning the stochastic dynamics of biological matter

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Abstract

The dynamics of biological systems, from proteins to cells to organisms, is complex and stochastic. To decipher their physical laws, we need to bridge between experimental observations and theoretical modeling. Thanks to progress in microscopy and tracking, there is today an abundance of experimental trajectories reflecting these dynamical laws. Inferring physical models from imperfect experimental data, however, is challenging and currently remains a bottleneck to data-driven biophysics. In this talk, I will present a set of tools developed to bridge this gap and permit robust and universal inference of stochastic dynamical models from experimental trajectories that are short, partial and noisy. They permit the efficient inference of dynamical models for overdamped and underdamped Langevin systems, as well as the inference of entropy production rates. I finally present early applications of these techniques, as well as future research directions.



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Nanopore-based analysis of modifications on human mRNAs to discern biological function

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Abstract

Mammalian cells expend large amounts of energy into generating >100 different enzymemediated RNA chemical modifications that can change the base-pairing, RNA secondary and tertiary structures, or recruitment of RNA binding proteins among many functions. Pseudouridine modified mRNAs are more resistant to RNAse-mediated degradation and have the potential to modulate immunogenicity and enhance translation in vivo. However, we have yet to understand the precise biological function of pseudouridine on mRNAs due to a lack of tools for their direct detection and quantification.

We have recently developed an algorithm for identifying pseudouridylated sites directly on mammalian mRNA transcripts using nanopore sequencing¹. We achieve this by exploiting systematic base-calling errors that occur at pseudouridylated sites as a function of deviations in the current signals for k-mers compared to an unmodified transcirptome² as well as long, synthetic mRNA controls bearing pseudouridines^{3,4}. We have created an important list of "ground truth", pseudouridylated sites, and have also uncovered previously unreported, pseudouridylated sites. We then use our algorithm to classify types of pseudouridine hyper-modification that may occur on mRNAs: Type 1 is mRNA sites with high occupancy; type 2 is mRNAs that may have >1 pseudouridine sites in the human transcriptome may be conserved or differentially expressed across cell types⁵, 2. Multiple modifications may be found on the same k-mer within a given mRNA, 3. A simple steady-state enzyme-substrate model reveals a strong correlation between psi synthase and mRNA substrate levels and psi modification frequencies⁶. and 4. Pseudouridine modifications are dynamically regulated in response to changes in cellular state (i.e., differentiation and exposure to environmental toxins)⁶.

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Engineering an implantable biohybrid nerve model towards synaptic deep brain stimulation

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Abstract

Available deep brain stimulation electrodes suffer from low stimulation resolution, low biocompatibility and limited coverage of the targeted tissue. To overcome those limitations, we propose a novel living biohybrid neural interface with the goal of restoring functional vision in the blind without a healthy optic nerve. Our interface uses living on-chip grown retinal neurons as relays to convert electrical signals from a stretchable microelectrode array into synaptic stimulation of a neural target tissue.

Our interface is based on a stretchable micropatterned microelectrode[1,2] array onto which we align axon guiding microfluidic structures that enable unidirectional guidance and merging of axons to form an artificial optic nerve. We increase the biocompatibility of our device by replacing the Polydimethylsiloxane (PDMS) based nerve forming channel with a collagen or gelatin methacryloyl (GelMA)[3] tube that is only 300 μ m in diameter and directly integrated onto the PDMS device.

We demonstrate the seeding of retinal spheroids into our biohybrid devices using a modified fluid force microscope. The retinal ganglion cells form an artificial optic nerve up to 3mm long that can transit from the device into the PDMS-bound hydrogel tube to reinnervate a matrigelbased target structure *in vitro*. We show that we can stimulate individual retinal spheroids using our stretchable microelectrode array. We also present *in vitro* data on how spikes propagate within the biohybrid implant using CMOS multielectrode arrays. Finally, we present first progress towards *in vivo* implantation.

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Towards a quantitative understanding of how viruses and vesicles interact with cells

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Abstract

Advances in optical microscopy have opened many exciting doors to more quantitative studies in biochermisty and cell biology because they allow one to detect and track individual nanoparticles and molecules. Although fluorescence microscopy remains work horse, it confronts several limitations, which have motivated many groups to develop fluorescence-free methods. Among various contrast mechanisms, scattering offers unique opportunities. About two decades ago, we showed that single gold nanoparticles as small as 5 nm could be detected via interferometric detection of their scattering, coined iSCAT [1]. Since then, it has been shown that unlabeled nano-objects such as proteins and viruses as small as 10kDa [2] can be detected, counted and tracked using iSCAT. We will discuss the application of this method in characterizing extracellular vesicles and cellular secretomes [3]. Furthermore, I will show that confocal iSCAT microscopy can achieve three-dimensional label-free imaging of cellular events such as the endoplasmic reticulum and microtubule dynamics as well as virus diffusion [4]. In addition, I will present a novel approach for controlled delivery of nanoparticles and small molecules to welldefined positions on a cell [5]. By combining these methods with conventional fluorescence microscopy, we establish a platform for studies of the way cells interact with extracellular particles with impact on a quantitative understanding of both infection and drug delivery. If time permits, I will also state a few words about a new optofluidic antenna that enhances singlemolecule detection in a solution, e.g., for FCS and FRET studies [6].

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TIBiSSe: A Textbook Dirac Semimetal

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Abstract

TlBiSSe is a 3D Dirac semimetal existing at the frontier between a topological insulator TlBiS₂ and a trivial insulator TlBiSe₂ [1-2]. It is a rare semimetal with a "clean" band structure, showing only a single, isolated conical band in a broad energy range, almost 0.5 eV around the Fermi level [3]. I will present a comprehensive description and a full investigation of this 3D Dirac semimetal at different doping levels, by combining infrared and magneto-optical spectroscopy measurements, together with ab-initio and analytical calculations. Both experimental and theoretical analyses reveal unequivocal signatures of 3D Dirac cones in optical and magneto-optical properties. These findings were enabled by precisely controlled crystal synthesis, which positioned the Fermi level near the Dirac point. This study highlights TlBiSSe as a material of choice for experimental studies of relativistic-like phenomena in solid-state physics [4].



Figure 1. First derivative of the relative magneto-transmission, and the orange dash line show the fit of the inter-Landau level excitations.

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Signatures of topological superconductivity in Josephson junctions

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Abstract

Topological superconductors represent a fruitful playing ground for fundamental research as well as for potential applications in fault-tolerant quantum computing. Especially Josephson junctions based on topological superconductors remain intensely studied, both theoretically and experimentally. The characteristic property of these junctions is their 4π -periodic ground-state fermion parity in the superconducting phase difference.

Using such topological Josephson junctions, we introduce the concept of a topological Josephson heat engine. We discuss how this engine can be implemented as a Josephson–Stirling cycle in topological superconductors, thereby illustrating the potential of the intriguing and fruitful marriage between topology and coherent thermodynamics. It is shown that the Josephson–Stirling cycle constitutes a highly versatile thermodynamic machine with different modes of operation controlled by the cycle temperatures. Finally, the thermodynamic cycle reflects the hallmark 4π -periodicity of topological Josephson junctions if fermion parity is conserved [1].

Moreover, we propose that phase-dependent measurements of the heat capacity offer an alternative to Josephson-current measurements to demonstrate key topological features. Even in an equilibrium situation, where the fermion parity is not conserved, the heat capacity exhibits a pronounced double peak in its phase dependence as a signature of the protected zero-energy crossing in the Andreev spectrum. This double-peak feature is robust against changes of the tunneling barrier and thus allows one to distinguish between topological and trivial junctions [2]. Although explicitly calculated for a short QSH-based Josephson junction, our results are also applicable to long as well as nanowire-based topological Josephson junctions.

Finally, we discuss thermal transport in Josephson junctions based on three-dimensional topological insulators. We compute the thermal conductance transverse to the direction of the superconducting phase bias and predict it to be universally quantized by half the thermal conductance quantum at phase difference π . This is a direct consequence of the parity-protected counterpropagating Majorana modes which are hosted at the superconducting interfaces [3].

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Evidence for multiple Andreev reflection in normal metal-superconducting-superconducting single-electron transistors

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Abstract

Coulomb blockade (CB) is an archetypical manifestation of charge quantization, which occurs in the electronic transport across a small metallic island [1]. CB can be suppressed by both classical and quantum fluctuations of the charge [2]. Classical charge fluctuations originate from thermal activation over an energy barrier, provided by the charging energy $E_C=e^2/2C$, with *C* the total capacitance and e the elementary charge. The quantum fluctuations can be described using the Landauer-Büttiker picture using individual conductance channels, with transmission probabilities τ , connecting the island to the leads [2]. In the case of normal-metallic (N) leads, the CB phenomena vanish when the transmission of at least one channel becomes equal to 1 in a Coulomb-blockaded island in a single-electron transistor (SET) [3].

For mesoscopic transport processes involving superconducting (S) leads, the energydependent quasiparticle (QP) spectrum has a gap Δ , which strongly inhibits tunneling at low energies and small τ [4]. At larger τ , multiparticle superconductive transport [4-6] comes into play. These processes can be either coherent, in the form of Josephson transport of Cooper pairs without voltage drop, or they may be dissipative, as multiple Andreev reflection (MAR) of order *m*, which sets in above a bias voltage threshold $eV=2\Delta/m$. MAR and Coulomb blockade (CB) are competing phenomena in superconducting single-electron transistors: While MAR fosters changing the number of island excess charges also with more than one elementary charge, CB suppresses such processes at small bias voltages [1-3]. Despite substantial experimental effort over the years [7-9], up to now no unambiguous evidence for MAR processes in superconducting CB devices has been reported.

In this talk I will be resent a novel device, a single-electron transistor with one superconductor-superconductor (SS) junction and a superconductor-normal metal junction (SN), called the SSN-SET [10]. The SS junction is realized as a mechanically controllable break junction (BJ), such that different conductance regimes and coupling strengths can be studied in the same device, while the SN junction is a classical oxide tunnel barrier (TB) with fixed properties (see Fig. 1). We find clear evidence for the presence of MAR processes in the current-voltage characteristics, both in the subgap regime as well as for bias voltages where single-quasiparticle tunneling is possible and MAR is suppressed in single junctions [11]. Furthermore, we observe that signatures of CB may reoccur at high bias while they are absent for small bias in the strong-coupling regime [3]. Our experimental findings agree with simulations using a rate equation approach in combination with the full counting statistics of MAR [11].

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Figure 1. Scanning electron microscope picture of a SSN-SET with a break junction (BJ) as one of the tunnel junctions in series with a superconductor—normal-metal tunnel barrier (TB), and the area in the middle (island) being capacitively coupled to a gate electrode.

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Mechanical writing of conductive lines on the nanoscale

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Abstract

Nanoscale conducting pathways, including naturally emerging ones such as conducting ferroelectric domain walls as well as artificially created ones, can act as functional building blocks for future nanoelectronics. Therefore, approaches to generate nanoscale conducting pathways are of high interest.

In the novel cluster Mott insulator GaV_4S_8 , we show that ferroelectric domain walls have highly enhanced conductivity with respect to the bulk. Using low-temperature scanning probe microscopy, we correlate surface topography with local conductivity and demonstrate that the conductivity enhancement is due to local strain gradients building up in the vicinity of the walls [1]. To establish this strain-driven mechanism, we successfully created conductive lines by scratching the surface using a cantilever with a diamond tip. Importantly, such artificial lines are not subject to crystallographic constraints, unlike domain walls. Owing to the multiferroic nature of the host compound, the ferroelectric domain walls can be mobilized both by electric and magnetic fields, which is a prerequisite for reconfigurable nanotechnology applications [2]. This strain-driven approach represents a new path for creating conductive nanowires and is generally expected to work in systems whose band structure is sensitive to strain gradients.



Figure: Conductive lines carved on the (111) surface of a GaV4S8 crystal using a cantilever with a borondoped single crystalline diamond tip. Left panel: surface topography recorded by a cryogenic AFM at 30 K. Right panel: Surface conductivity map over the same area recorded via conductive-AFM at 30 K.

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A brief history of spectroscopic manifestations of the Kondo effect

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Abstract

In 1930, a resistance minimum observed in dilute magnetic alloys [1,2], was the first experimental evidence for a new scattering mechanism of conduction electrons at magnetic impurities at low temperatures. More than 30 years later, J. Kondo developed a theory which described the effect as a consequence of the spin-flip scattering of conduction electrons at a localised magnetic moment [3,4]. About the same time P. W. Anderson developed a "single impurity model" [5] where he calculated the implications of this scattering mechanism for the local density of electronic states. This conjecture triggered numerous experimental physicists to search for and finally to discover this resonance in transition metal, rare earth elements and in their alloys using techniques such as photoelectron, point contact, electronic transport, and scanning tunneling spectroscopies (STS). The latter technique revealed the presence of Kondo resonances also in molecular systems containing unpaired electron spins. These discoveries opened the door for a detailed study of electronic transport and molecular magnetism on the molecular scale.

Recently, a magnetic sensor has been fabricated by attaching a single nickelocene molecule to the tip apex of a scanning tunneling microscope (STM) [6,7]. Similarly, a tip that has its apex functionalized with a Kondo screened spin system, a small Ce cluster [8], senses the spin (S = $\frac{1}{2}$) of an individual Ce adatom adsorbed on a Cu₂N ultrathin film (no external magnetic field). This functionalised tip is used as a spin detector. The technique may lead to applications in ultra-dense magnetic storage, spintronics computers, and quantum information technologies.

Surprisingly, a new view on the origin of zero-bias anomalies of Co atoms atop noble metal surfaces, as detected by STS, emerged: "These features originate from gapped spin-excitations induced by a finite magnetic anisotropy energy, in contrast to the usual widespread interpretation relating them to Kondo resonances" [9]. Experimental evidence for the existence of these theoretically predicted "spinarons" in Co adatoms has been reported [10].

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Experimental Routes for Realization of Topological Josephson Junctions

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Abstract

Majorana bound states, which are their own antiparticles, are predicted to emerge as zeroenergy modes localized at the boundary between a topological superconductor and a topologically trivial region. Unlike BCS superconductors, nature has not provided us unambiguous topological superconductors. However, it was realized that by interfacing BCS superconductors and semiconductors with strong spin--orbit coupling [1] it is possible to create a system that can host topological states. Hence epitaxial superconductors and semiconductors have emerged as an attractive materials system with atomically sharp interfaces and broad flexibility in device fabrications incorporating Josephson junctions [2]. We discuss the basics of topological superconductivity and provide insight on how to go beyond current state-of-the-art experiments [3]. We argue that the ultimate success in realizing Majorana bound state physics relies on the observation of non-trivial fusion and braiding experiments [4].



Figure 1. Super-Semi realizations of topological phases hosting Majorana fermions

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Excitonic insulator in atomic double layers

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Abstract

Excitonic insulators have been proposed as a solid-state platform for quantum many-boson physics. Although the concept of an excitonic insular has been understood for sixty years, it remains challenging to establish distinct experimental signatures of its realization. In this talk, I will discuss the development of transition metal dichalcogenide double layer structures (Coulomb-coupled MoSe₂/WSe₂ monolayers) and electrical injection of interlayer excitons up to 10^{12} cm⁻². We establish electrical control of the chemical potential of interlayer excitons and present thermodynamic evidence for an excitonic insulating phase by capacitance measurements [1]. The strong interlayer excitonic correlation also gives rise to perfect Coulomb drag [2]. By electrically tuning the hole density in WSe₂ to be two times the electron density in MoSe₂, we also generate equilibrium interlayer trions with binding energy about 1 meV at temperatures two orders of magnitude below the Fermi temperature [3].

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Chiral Electrokinetic Phenomena in Single Nanopores

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Abstract

The arrangement of solvent molecules and ions at solid-liquid interfaces determines electrochemical properties that are important in separation platforms, sensing technologies, and energy-storage systems. Here we show that single glass and polymer pores in contact with propylene carbonate (PC) solutions of LiClO₄ exhibit an effective surface potential that is modulated by the chiral form of the solvent. Electrochemical and electrokinetic measurements of ionic transport through glass pipettes and polymer pores revealed that the effective surface potential is significantly lower in solutions prepared using enantiomerically pure PC than in solutions prepared using racemic PC. Both pore systems became positively charged in all racemic solutions examined in the range of LiClO₄ concentrations between 1 mM and 100 mM, whereas solutions in (R)-PC induced a positive surface potential only at concentrations above ~ 5 mM. The effective surface potential is quantified through asymmetry in current-voltage curves and zetapotential measurements. Vibrational sum-frequency-generation experiments on LiClO₄ solutions in racemic and enantiomerically pure PC indicate that the surface bilayer in the former is more strongly organized than in the latter, dictating the favorable positions for lithium and perchlorate ions in each case. The more ordered molecular packing in the racemic liquid leads to accumulation of lithium ions on the outside of the bilayer, creating a higher effective positive charge. Our results highlight the extreme sensitivity of the interfacial potential on molecular organization of the solvent, and the relatively unexplored role that chirality can play in electrokinetic phenomena. The talk will also present our newest results on preparation of interacting ionic circuits.

Fingerprints of low-energy scattering in the superconducting state

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Abstract

The anomalous properties of many correlated metals of current interest are believed to be caused by singular low-energy scattering processes. The latter should be most clearly observable in the limit of low temperatures. However, in this limit, the situation is often complicated by the transition of the metal to the superconducting state. Motivated by this state of affairs, we search for experimentally observable fingerprints of low-energy scattering processes in superconductors.

We will introduce our recent work^[1] dealing with the interplay between inelastic processes, described within the self-consistent Born approximation, and elastic scattering on strong magnetic disorder, treated within the coherent-potential approximation. Using the resulting Eliashberg-like formalism, we have shown that the tunneling density of states at low energies can be characterized by the Dynes formula with the pair-breaking parameter Γ . We will discuss how the temperature dependence of Γ could possibly be used to extract information about inelastic processes in the limit of low energies.

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Nitride-based superconducting devices on sapphire for quantum computing

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Abstract

The quest for advanced superconducting devices for quantum computing has spurred numerous proposals aimed at enhancing coherence times. Nitride-based superconducting devices have emerged as a promising platform for the next generation of quantum computing, thanks to their stability and favorable superconducting properties.[1] Utilizing reconstructed $\sqrt{31} \times \sqrt{31}$ R±9° *c*-plane sapphire as a substrate offers significant benefits for these devices, combining long-range atomic order with a low dielectric loss tangent.[2,3] Thus, integrating reconstructed sapphire with superconducting nitride films promises the development of superior superconducting devices.

In this study, we present the fabrication of all-nitride superconducting devices, specifically TiN/AlN/TiN Josephson Junctions, deposited via molecular beam epitaxy on c-plane sapphire. These devices demonstrate high crystalline quality and exceptional superconducting properties, making them ideal candidates for quantum computing applications. When combine with stencil mask technology for selective area growth, the potential for quantum circuits with no post-growth etching of the device is realised.[4] We examine the advantages of these devices over commonly used alternatives and discuss how reconstructed sapphire contributes to optimal growth characteristics.

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Capturing the mechanosensitivity of cell proliferation and its effects on tissue development

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Abstract

Despite the primary role of cell proliferation in tissue development and homeostatic maintenance, the interplay between tissue structure, cell mechanoresponse, and cell growth and division is not yet understood. I will address this issue by reporting on an experimental investigation of cell proliferation on all time- and length-scales of the development of a model tissue, grown on collagen-coated glass or deformable substrates. Through extensive data analysis, we demonstrate the relation between mechanoresponse and probability for cell division, as a function of the local cell density. I will, furthermore, discuss a minimal model of cell division in tissue environment that can recover the data. By parameterizing the growth and the dividing phases of the cell cycle, and introducing such a proliferation model in dissipative particle dynamics simulations, we recover the mechanoresponsive, time-dependent density profiles in 2D tissues growing to macroscopic scales. The importance of separating the cell population into growing and dividing cells, each characterized by a particular time scale, is further emphasized by calculations of density profiles based on Fisher-Kolmogorov equations adapted by introducing a delay. Together, these results show that the mechanoresponse on the level of a constitutive cell and its proliferation results in a matrix-sensitive active pressure. The latter evokes massive cooperative displacement of cells in the invading tissue and is a key factor for developing largescale structures in the steady state.

Light-sheet imaging of cleared mouse brains

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Abstract

The central nervous system (CNS) relies on intricate interactions among large populations of neurons across different areas. To comprehend the complex processes and functions of the CNS, there is a growing demand for imaging techniques that provide access to the neuronal activity of large networks with exceptional spatiotemporal resolution. Light sheet fluorescence microscopy (LSFM) has emerged as a highly promising optical sectioning technique, enabling volumetric imaging across multiple length scales while maintaining high spatial resolution and minimizing photobleaching and phototoxicity [1, 2]. One of the main challenges of using LSFM for imaging whole mouse brains is the need for tissue clearing. Tissue clearing techniques involve treating biological samples with chemical solutions to reduce opacity and make them transparent, while preserving their original structure which allows for deep imaging of the entire specimen. We use whole-brain organic solvent based clearing protocols, such as iDISCO. Samples cleared in this manner can then be imaged using LSFM and aligned to a mouse brain atlas, providing a map of all the different brain regions. By combining this methodology with different experimental paradigms that cause the expression of fluorescent proteins in the mouse brain we hope to be able to study neural circuits involved in sensorimotor learning.

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Over 30-Fold Enhancement in DNA Translocation Dynamics through Nanoscale Pores Coated with an Anionic

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Abstract

Solid-state nanopores (ssNPs) are single-molecule sensors capable of label-free quantification of different biomolecules, which have become highly versatile with the introduction of different surface treatments. By modulating the surface charges of the ssNP, the electro-osmotic flow (EOF) can be controlled in turn affecting the in-pore hydrodynamic forces. Herein, we demonstrate that negative charge surfactant coating to ssNPs generates EOF that slows-down DNA translocation speed by >30-fold, without deterioration of the NP noise, hence significantly improving its performances. Consequently, surfactant-coated ssNPs can be used to reliably sense short DNA fragments at high voltage bias. To shed light on the EOF phenomena inside planar ssNPs, we introduce visualization of the electrically neutral fluorescent molecule's flow, hence decoupling the electrophoretic from EOF forces. Finite elements simulations are then used to show that EOF is likely responsible for in-pore drag and size-selective capture rate. This study broadens ssNPs use for multianalyte sensing in a single device.



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Dielectric properties of liquids confined in atomically thin nanochannels

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Abstract

Water is a central molecule to diverse natural phenomena and technologies, from ionic exchange between cells in our bodies, to electrolysis at the interface of electrodes in batteries. Interfacial water and the way is behaves differently to bulk has been of particular interest for the past century. This thesis investigates the electrodynamic and dielectric properties of interfacial water, by confining it in nanochannels as thin as 1nm made with van der Waals crystals assembly. The possibility to fabricate such channels has led to a number of discoveries relating to the molecular behavior of liquids[1]. Using the Scanning Dielectric Microscopy (SDM) technique[2] which probes dielectric properties on the atomic scale, Fumagalli et al were able to measure the suppressed out-of-plane dielectric constant of interfacial water[3] confined in nanochannels made with graphite and hexagonal Bohron-Nitride (hBN). This thesis is the continuation of that study, investigating the in-plane contribution of the dielectric properties of thin water films. We have found that water confined in hBN nanochannels exhibit an anomalously high in-plane dielectric response. Using meausrements on a wide array of frequencies, we show that this is due to high in-plane conductivity and dielectric constant in interfacial water.

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Clarifying the nature of the covalent bond

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Abstract

Understanding the nature of the chemical bond is of fundamental importance. In this respect, we have generalized and solved exactly the extended Heitler-London model for H_2 and related two-atomic molecules, ranging from H_2 and HeH⁺ to ionic LiH [1] systems. It turned out that determining exactly the covalent and ionic relative contribution is not sufficient to characterize the bonding, as the covalency becomes maximal in the limit of separated atoms (the dissociation limit). The reason for this unphysical feature appears when the particles are regarded as *indistinguishable*, whereas in the limit of separated atoms they are *distinguishable*. To cure that we introduced *the atomicity* and have defined *the true covalency*. The resultant bonding factors are depicted in Fig. 1a as a function of interatomic distance R. Two novel features appear. First, a crossover boundary between the normal and Mott-Hubbard-type regimes, in which the interelectron repulsive interaction dominates over kinetic energy. The second of them is the von Neumann entropy identified as the entanglement correlation, shown in Fig. 1b and compared with the bonding factors. In effect, the bonding can be characterized by either true covalency and ionicity combined together or by the entanglement correlation.

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Figure 1. (a) The bonding factors as a function of interatomic distance R; the shaded area marks the Mott-Hubard regime. (b) Comparision of combined bonding factor with the von Neumann entropy; inset: true covalency (blue) and ionicity (green) compared to the von Neumann entropy (purple)

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Nematic superconductivity in twisted bilayer graphene

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Abstract

Typical moiré systems consist of 10,000 atoms per unit cell, however, as mainly the emerging flat bands determine the novel correlated and topological phases, an effectiv density-matrix related to the flat bands usually suffices to describe the main physics. The correlated insulator phases of magic angle bilayer graphene at even integer filling factor, e.g., can be characterized by an U(4)-ferromagnet. But this approximate symmetry is broken in real samples and the way how it is broken may lead to the yet unexplained asymmetry between the superconducting phases for electronic and hole doping.

In order to address the phase diagram of realistic moiré systems, I will thus start from a microscopic tight-binding model for twisted bilayer graphene (TBG) within the Hartree-Fock approximation and present two ways how to reduce the full density matrix to a density matrix based on a SU(4)-symmetry [1,2,3]. We find that at charge neutrality point also the reduced density matrix is described by a pure (valley coherent) state. We further find nematic superconductivity with valley polarization for hole doping, see Figure 1, and valley coherence for electron doping, see Figure 1 and Reference [3].

Finally, I outline our theory of Ising superconductivity of twisted trilayer graphene [4] and show how real-space chirality can be measured in linear transport experiments [5].



Figure 1. Energy contour maps showing the Fermi lines in the second valence band for (A) spin-up and (A') spin-down electrons in the moir/'e Brillouin zone of TBG for filling fraction of 2.4 holes per moiré unit cell. Contiguous contour lines differ by a constant step of 0.02 meV, from lower energies in blue to higher energies in light color. (B) Energy contour maps showing the Fermi line in the second conduction band at filling fraction of 2.3 electrons per moiré unit cell.

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Identifying topological superconductivity using Tomasch oscillations

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Abstract

The identification of topological superconductors usually involves searching for in-gap modes that are protected by topology. However, in current experimental settings, the smoking-gun evidence of these in-gap modes is still lacking – partially due to difficulties in distinguishing them from disorder effects.

In this work, we propose to support the distinction between two-dimensional conventional s-wave and topological p-wave superconductors by above-gap transport signatures [1]. Our method utilizes the emergence of Tomasch oscillations [2] of quasiparticles in a junction consisting of a superconductor sandwiched between two metallic leads, see Figs. 1(a) and (b). We demonstrate that the behaviour of the oscillations in conductance as a function of the interface barriers provides a distinctive signature for s-wave and p-wave superconductors, see Fig.1(c). Specifically, the oscillations become weaker as the barrier strength increases in s-wave superconductors, while they become more pronounced in p-wave superconductors, which we prove to be a direct manifestation of the pairing symmetries. Our method can serve as a crucial complementary probe for identifying some classes of topological superconductors through the above-gap transport.



Figure 1. (a) Sketch of the NSN junction consisting of a superconductor (S) coupled to two normal metal

leads (N) with the interface barrier Z. (top panels) The quasiparticle dispersion for $k_y = 0$ in all three regions. (b) Differential conductance as a function of energy for both the *s*- and *p*-wave superconductors in the absence of barriers (Z = 0) [3]. (c) Same as (b) in the presence of finite barriers with equal strengths Z = 4. Grey arrows denote the extremal points of a single oscillation.

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Insights into local oxygen reorganization in hafnia-based ferroelectric films

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Abstract

The discovery of ferroelectricity in nanoscale films of binary oxides, particularly hafnia, has reignited interest in understanding the emergence of ferroelectric properties at the nanoscale. The unusual size scaling of polarization in these films is a focus of intense investigation. Given the sensitivity of polarization in hafnia-based films to the oxygen content, it has been hypothesized that polarization switching is intertwined with electrochemical reactions. Though these processes have been shown to co-occur, their relationship remains unclear. We conducted direct observations of the electrochemical state within regions exhibiting preset polarization directions in hafnia-based ferroelectric films, employing hard x-ray photoelectron spectroscopy (HAXPES). Our findings reveal more pronounced electrochemical changes in films with lower polarization, suggesting a lack of direct linkage between polarization and electrochemical changes. These results mark progress in unraveling the origins of the ferroelectric response in hafnia-based films.

Cuprates, Pnictides, and Sulfosalts: Lessons in Functional Materials

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Abstract

Murunskite K2FeCu3S4 is a representative sulfosalt isostructural to the pnictides, but with electronic properties more similar to the insulating parent compounds of the cuprates [1]. Here it is used as a bridge to compare the chemical and physical roles of metal and ligand orbitals in cuprates and pnictides.

In cuprates, I will argue that ionicity, covalency, and metallicity are tightly interwoven to give rise to high-temperature superconductivity (SC). Their most remarkable property is the interaction of an ionically localized hole in the Cu-O 3d-2p bond with a Fermi liquid metallized via the Cu-O 4s-2p bond, which is critically important for the superconducting mechanism [2]. In the pnictides, the ionic and metallic sectors are separate. The former sets the lattice spacing via the Fe 3d e_{2g} orbitals binding the ligands, and the second proceeds via direct 3d t_{2g} orbital overlaps between the iron atoms, in which superconductivity is found together with significant magnetic correlations [3]. In murunskite, the greater covalency of sulfur orbitals compensates for total disorder in the Fe atom positions, giving rise to an agglomeration of fractal magnetic clusters coexisting with perfect crystallographic order and exhibiting a surprisingly robust antiferromagnetism (AF) [4]. Because the open ligand orbitals play an important role in it, the essentially local AF of murunskite is more similar to the SC of the cuprates than to the AF of the pnictides, in which the ligands are passive.

On the basis of these examples, it is argued that the development of next-generation paradigms in functional materials must treat the physical and chemical roles of atomic orbitals on an equal footing. These meet in the dual role of the chemical potential, which simultaneously accounts for the level density of metallic carriers and for the balance of chemical reactions between constituents in the solid state. A recent insight into the physical limitations of the Hohenberg-Mermin-Wagner theorem for both magnetism and SC [5] is encouraging for the fabrication of 2D materials and heterostructures to harness such understanding.

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A multimodal approach to uncovering magnetic symmetries: the case of EuIn₂As₂

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Abstract

Understanding and manipulating emergent phases, which are themes at the forefront of modern quantum materials research, rely upon correctly identifying underlying symmetries. This general principle has been particularly prominent in materials with coupled electronic and magnetic degrees of freedom, in which magnetic symmetries can cause drastic changes to electronic states, including protecting exotic topological phases. EuIn₂As₂ is a prominent example of the latter: it has been identified as a prime candidate to host the elusive axion state [1,2]. However, despite intense experimental efforts, no direct evidence for topology in EuIn₂As₂ is available, motivating a reexamination of standard assumptions.

I will show how combining scattering data with bespoke spatially-resolved symmetrysensitive optical experiments and a group theory analysis led us to uniquely identify the two magnetic phases in EuIn₂As₂ [3]. While our data contradict previous proposals for magnetic structures, we demonstrate that all experimental results on EuIn₂As₂ can be reconciled into a unique picture. In addition to revealing the causes and consequences of exotic magnetism in EuIn₂As₂, I will highlight the importance of combining the information obtained through complementary experimental probes, with special emphasis on probes of time-reversal symmetry breaking. I will argue that such a multimodal approach is an invaluable asset in the quest for determining symmetries of complex ordered phases in a broad class of materials.

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Effect of Charge Doping on the Electronic Structure of Strongly Confined Graphene Quantum Dots

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Abstract

A dramatic increase of interest in perovskite materials in recent years has been driven primarily by a discovery that a subset of these materials, halide-perovskites (HPs), possess combination of properties excellent for exploitation in photovoltaics, LEDs, lasers, optical and radiation detectors and other technologies. Despite the promise of HPs, their limited thermal and chemical stability and inclusion of toxic ions, such as lead, pose challenge for their commercial exploitation. Chalcogenide perovskites (CPs), crystalline solids with the composition ABX₃, where A, B, are metal cations and X = S, Se, have been recently suggested as a possible alternative to the structurally related HPs. Theoretical and early experimental studies indicate that CPs have electronic properties similar to the HPs, are comparable or better light absorbers, have better chemical and thermal stability and can be prepared without the use of toxic elements. However, experimental studies of the CPs have so far been limited, mainly due to the challenges with their preparation. In the talk I will summarize our progress in development of synthetic methods for preparation of CPs and quantitative comparison of the thermal stability of HPs and CPs. I will also discuss the results of our Molecular Dynamics modelling of the effect of temperature on physical and electronic structure of CPs.

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Genomes as documents of evolutionary history

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Abstract

Biology is a historical science. The structure of biological systems, from molecules to ecosystems, is the result of a long evolutionary process that began over 3 billion years ago. The idea that studying the pattern and process of evolution is the key to understanding living systems is now becoming widely accepted.

Zuckerkandl and Pauling asked the question where in living systems has the greatest amount of their past history survived and how it can be extracted? Their answer, that best fit are the different macromolecules that carry genetic information — what today we would call genomic sequence data, gave rise to molecular phylogenetics. Coupled with extraordinary advances in DNA sequencing, molecular phylogenetics has allowed us to reconstruct increasingly accurate and better resolved evolutionary trees that have revolutionised our understanding of the evolution of Life on Earth.

Yet, the information contained in genomes goes beyond the historical. Genomes also encode information on organismal complexity — an organism's developmental plan and functional program, no matter how complex, is contained in the genome. In the last ten years, I have been developing methods that model the evolution of genomes by integrating events of gene duplication, gene loss, and lateral gene transfer in the simultaneous reconstruction of species and gene histories. These methods yield much better estimates of the gene content of ancestral genomes, opening the door to accurate reconstructions of ancestral species characteristics.

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Electronic subsystem duality: a key factor in cuprate superconductivity

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Abstract

Understanding the intricate physical properties of unconventional superconductors, alongside other correlated materials, remains a formidable scientific endeavor. This challenge arises from significant shifts in electronic structure and Coulomb interactions among electrons, leading to diverse phase formations influenced by varying dopant levels and temperature. In the presentation, I will provide an in-depth exploration of the phenomenology and microscopic characteristics of copper-oxide superconductors (cuprates), with a specific focus on the universal features observed in electrical [1,2] and optical [3] conductivity, shedding light on the presence of two distinct electronic subsystems. Our analysis reveals that the overall electronic configuration comprises charges 1+p, where p denotes the dopant level. At low carrier concentrations, precise localization of one hole per unit cell is observed; however, with increasing doping and temperature, this hole gradually transitions into an itinerant state. Remarkably, itinerant holes consistently exhibit Fermi liquid behavior across the phase diagram of copperoxide superconductors. Furthermore, we observe that the charge localization associated to the decrease of the density of states at the Fermi surface, results in the formation of disconnected Fermi-arcs, but is not a consequence of a true Fermi surface reconstruction driven by a phase transition [2]. Conclusively, we propose a plausible superconductivity mechanism, which aligns with pivotal experimental observations, emphasizing the interaction between Fermi-liquid carriers and localized holes. Furthermore, we leverage the transition in microscopic chemical bonding from ionic to covalent within the copper-oxygen planes to elucidate the phase diagram of these captivating compounds.

We acknowledge the support from the National Science Centre, Poland, Grant No. OPUS: 2021/41/B/ST3/03454, and from the "Excellence Initiative–Research University" program for AGH University of Krakow.

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From Solid State to AstroParticle Physics: Search for dark-matter axions

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Abstract

The nature of the dark matter in the Universe is one of the most compelling questions in all of science. Dark matter makes up roughly 85% of the Universe's mass and we do not know what it is. It has gravity, but otherwise interacts extremely weakly with ordinary matter, making detection very challenging. The axion, a very well-motivated candidate for the dark matter, can be detected by conversion to microwave photons in a strong magnetic field. This process, invented 40 years ago by my colleague Pierre Sikive, is the basis of almost all axion searches. In the late 1980s, a group at Florida built a detector to search for axions within the dark-matter halo of our Galaxy. The design of this experiment, including cavity configuration, materials, cavity tuning, data acquisition method, and data analysis techniques were used by subsequent detectors, eventually becoming the Axion Dark Matter eXperiment (ADMX). Results will be described from the "Generation 2" ADMX detector, an axion search sensitive to the high-priority models of axions as dark matter. The improvements allowing ADMX to reach this position were the incorporation of a high-performance dilution refrigerator and an ultrasensitive SQUID microwave amplifier, giving noise backgrounds in the 100 mK temperature range. The remaining components are a large-volume superconducting magnet and a high-Q tunable microwave cavity. All components are things that are familiar to persons doing solid-state, low-temperature research.

Collective phenomena in disordered systems: A nonperturbative functional renormalization group approach

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Abstract

The interplay of interactions and quenched disorder in condensed-matter systems may lead to a multiplicity of low-energy metastable states, a phenomenon that often gives rise to slow or glassy dynamics, aging and hysteresis. Evolution between these states then involves collective singular events in the form of avalanches at zero temperature or rare events in the form of droplet excitations at nonzero temperature. Such events cannot be treated by standard theoretical methods such as mean-field and perturbation theory. Describing the large-scale physics requires a nonperturbative and functional Renormalization Group approach. This will be illustrated by the resolution of several long-standing puzzles associated with a paradigmatic disordered model, the random-field Ising model, both in equilibrium and out of equilibrium. Finally, extension of the approach to other problems will be discussed.

Stalactite HfO₂ Nanopore for Osmotic Energy Conversion

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Abstract

Nature provides a wide range of self-assembled structures from the nanoscale to the macroscale. Under the right thermodynamic conditions and with the appropriate material supply, structures like stalactites, icicles, and corals can grow. However, the natural growth process is time-consuming. This work demonstrates a fast, nature-inspired method for growing stalactite nanopores using heterogeneous atomic deposition of hafnium dioxide at the orifice of templated silicon nitride apertures. The stalactite nanostructures combine the benefits of reduced sensing region typically for 2-dimensional material nanopores with the asymmetric geometry of capillaries, resulting in ionic selectivity and stability. Moreover, the HfO₂ anisotropic growth is not confined to single nanopores but extends to multi-pore silicon nitride membranes with small variations in pore size. This observation underscores the high scalability potential of the approach. This proposed growing method provides an adaptable nanopore platform for basic and applied nanofluidic research, including biosensing, energy science, and filtration technologies.



Figure 1. a) Stalactites and stalagmites: Artist's representation of the natural formations b) Electron microscopy (EM) micrographs of HfO2 stalactite nanopores on the templated silicon nitride apertures obtained in this study. The inset shows the TEM image of several nanopores. Scale bar, 500 nm. c) The growth procedure consists of the regular ALD and the selective templated aperture growth. d) Schematic 3D view of the stalactite nanopore.

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Optimizing nanopore signal acquisition and processing: implication for single molecule characterization of adeno associated viruses

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Abstract

The benefits of using nanopores as a tool for signal acquisition have nowadays been assessed in multiple fields of science, from biosciences, e.g. for the identification of single biological molecule translocations [1], or the analysis of folding and unfolding of DNA strands [2], to nanoparticle sensing, useful for the characterization of nanomaterials [3]. Within biosciences, it has been demonstrated how high sampling rates (allowing for high bandwidths), combined with an appropriate experimental setup (small and thin nanopores, high salt concentrations and voltages), dramatically improve the morphology of the translocation events recorded through a nanopore reader. In fact, Lin et al. [2] showed how data acquisition at 10MHz bandwidth allows for more reliable morphological features in terms of event amplitude, dwell time, and the identification of the multiple current steps which could constitute a single event. A potential use case for such high bandwidth measurement systems is the single molecule characterization of Adeno-Associated Viruses (AAVs), and in particular their genetic cargo. Recently, Karawdeniya et al. [1] demonstrated how a deep classifier, trained on chunks of AAV translocation signals, obtained good classification accuracy when discriminating AAV signals into empty, loaded with a single DNA strand, or with a double strand, although not at the single event level, as the used sampling rate amounted to 250kHz.

In Elements, we are currently testing how the bandwidth of a nanopore reader can actually impact the characterization of a single AAV particle translocation event, especially in terms of morphology. In fact, we observed that at a low sampling rate (e.g. 100kHz, corresponding approximately to 25kHz bandwidth) recorded events were made up of very few samples (e.g. 3 or 4), i.e. not sufficient for an appropriate morphological characterization, as observed in [2]. Our preliminary results confirm that increasing the sampling rate to 200kHz improves the resolution of the translocation dynamics, but we believe that event acquisition at even higher bandwidth (e.g. 1MHz) could offer us better morphologies, useful for a more accurate estimate of features usable for machine learning studies, thus pushing forward the results by Karawdeniya et al. [1]. One clear drawback of very high sampling rates is the huge amount of data produced, e.g. 1 sample every 25ns (80MB/s). Therefore, in Elements, we are also testing how to optimize the amount of saved data, implementing the real-time acquisition of the event traces only, instead of the full gap free current signal, thus saving storage space, without affecting the quality of the morphology of the single events. As a future development, we will start investigating the most promising event features (in addition to amplitude and dwell time) and classification techniques for direct firmware implementation, to enable real-time and accurate nanoparticle analysis, i.e. the content of AAV particles.

From Solid-State to Biophysics XI Dubrovnik (Croatia), 8-15 June 2024

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Nature-inspired materials for energy applications

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Abstract

Nature provides a wide range of self-assembled structures from the nanoscale to the macroscale. Under the right thermodynamic conditions and with the appropriate material supply, structures like stalactites, icicles, and corals can grow. However, the natural growth process is time-consuming. This work demonstrates a fast, nature-inspired method for growing stalactite nanopores using heterogeneous atomic deposition of hafnium dioxide at the orifice of templated silicon nitride apertures. The stalactite nanostructures combine the benefits of reduced sensing region typically for 2-dimensional material nanopores with the asymmetric geometry of capillaries, resulting in ionic selectivity and stability. Moreover, the HfO₂ anisotropic growth is not confined to single nanopores but extends to multi-pore silicon nitride membranes with small variations in pore size. This observation underscores the high scalability potential of the approach. This proposed growing method provides an adaptable nanopore platform for basic and applied nanofluidic research, including biosensing, energy science, and filtration technologies.



Figure 1. a) Stalactites and stalagmites: Artist's representation of the natural formations b) Electron microscopy (EM) micrographs of HfO2 stalactite nanopores on the templated silicon nitride apertures obtained in this study. The inset shows the TEM image of several nanopores. Scale bar, 500 nm. c) The growth procedure consists of the regular ALD and the selective templated aperture growth. d) Schematic 3D view of the stalactite nanopore.

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Emergent electromagnetic induction in skyrmion host and spin chiral matter

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Abstract

Intriguing electromagnetic phenomena show up in a solid when the electrons spins take a helical form. To name a few, the cycloidal order of spin moments can produce the electric polarization and realize the multiferroics where ferroelectric and magnetic orders coexist, enabling the cross control of magnetism with electric field. When spin helices hybridize with plural propagation directions, there emerge the topological spin textures, such as the lattice forms of magnetic field or Berry curvature acting on the conduction electrons and causing the gigantic topological Hall effect. Furthermore, the dynamics of these skyrmion or helical-spin textures, as excited by electric current flow, generates the emergent electric field acting on the electrons, *i.e.*, emergent electromagnetic induction. We argue the emergent induction phenomena related to the current-induced dynamic transitions of skyrmions and spin helices.

The surprising magnetism of murunskite

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Abstract

Exploring novel materials as the candidates for unconventional superconductors can help to understand the mechanism of this exotic phenomenon but also lead to synthesis of compounds with important technological applications. The main compound of interest is murunskite (K2FeCu3S4), a material isostructural to 122 iron-based superconductors, with iron and copper randomly distributed in the same metal site. Murunskite is an insulator with sulfur orbitals partially open and electronically active, similar to oxygen orbitals in cuprates.

Through comprehensive neutron, Mössbauer, and XPS measurements on murunskite single crystals, we unveil antiferromagnetic structure with a nearly commensurate quarterzone wave vectors. Intriguingly, the only identifiable magnetic atoms, iron, are randomly distributed over one-quarter of available crystallographic sites in 2D planes, while the remaining sites are occupied by closed-shell copper. Our findings align with a disordered-alloy picture featuring magnetic interactions up to second neighbors. Moreover, in the paramagnetic state, irons are in mixed valence states, associated with two distinct paramagnetic sites identified by Mössbauer spectroscopy. Upon decreasing the temperature below the appearance of magnetism, these two signals merge completely into a third, implying an orbital transition. It completes the cascade of (local) transitions that transform iron atoms from fully orbitally and magnetically disordered to homogeneously ordered in inverse space, but still randomly distributed in real space.

Finally, substitution and doping on all three crystallographic sites leading towards the metallization and superconductivity in the murunskite family will be shortly discussed.

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Charge density waves and Kondo physics in 2D van der Waals materials

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Abstract

Recent discovery of a 2D van der Waals (vdW) heavy fermion system, CeSiI, has opened some fundamental questions in the physics of quasi-2D materials with strong correlations. For example, if probed by charge transport, the carriers in CeSiI seem light, whereas in heat capacity, the carriers display heavy fermion character [1]. In another 2D vdW material, CeTe₃, that is also considered to host a Kondo physics [2], such behavior is highly unexpected, as this material also hosts very strong and incommensurate charge density waves (CDW) [3], thought to be incompatible with Kondo screening. In this talk, we will examine some of these problems by using angle resolved photoemission spectroscopy (ARPES). We will explore the typical prerequisites for CDW formation (Fermi surface nesting and electron phonon coupling) to show how their relative contribution affects the properties of CDW in 2D vdW materials. We will also demonstrate that in the materials containing cerium, the hybridization of highly itinerant states with the localized Ce 4*f* multiplet is the key for addressing the observed "light-heavy" dichotomy in Kondo systems.

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Response functions of correlated systems within Green's function theory

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Abstract

At its fundamental level, the physical properties of chemical, physical, and biological systems are governed by the underlying fundamental equations of motion. It is becoming increasingly possible to solve these equations with high fidelity, albeit for systems far smaller than biological ones. If solved, a great deal of insight into these systems is possible. This is especially important when 2-particle response functions are further calculated. The latter supply information about response of a system to external perturbations, e.g. dielectric response for charge, magnetic response for spin, and electron-lattice interation for lattice perturbations, and thus directly simulate many of the probes that characterize these systems.

Solutions of the Schrodinger equation can be classed according to the independent variable used to solve them: density in DFT (density functional theory), wave functions in quantumchemical (QC) methods, and Green's function methods. QC methods the king for accuracy, but they are expensive and restricted to small molecules; DFT is the most popular owing to its simplicity, but its scope and accuracy is limited. I will argue that Green's function methods are the "Goldilocks" approach: they can be high enough fidelity to approach QC methods, and they can scale much more efficiently with system size, making them practical for functional materials.

Moreover, Green's function methods generate these response functions as byproduct of the theory, and thus they hold promise for being a particularly powerful tool for most STEM fields. I will present some present work on these methods and illustrate them with examples of response functions that do an excellent job at simulating a wide range of experimental probes in a model-free way.

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Tunable electrochemical activity in ferroionic CeO2/BTO thin films

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Abstract

Ferroionic materials are heterostructures consisting of ferroelectric and ionic metal oxides [1]. This emerging class of multifunctional materials combines the individual properties of ferroelectricity with ionic-electronic conductivity and electrocatalysis. Moreover, they can generate unexpected properties, especially at the interface between the materials [2]. Electrocatalysis in ionics usually requires high energy above 100 kJ/mol, generally achieved at high temperatures (> 600 K) or additional precious catalysts and doping strategies [3]. However, pairing such catalysts with ferroelectrics with a built-in electric field promotes an efficient separation of charges. Cerium oxide CeO₂₋₈ (ceria) is an excellent candidate for its high temperatures, i.e. oxygen vacancies (V_0^-) and small polarons (Ce'_{Ce} , Ce³⁺ species) [4].

Here, we present the modulation of chemical properties in BaTiO₃/CeO₂ (BTO/ceria) heterostructures by controlling the polarisation direction (negative and positive) of the ferroelectric layer. Positive and negative fixed polarisation at the BTO thin film (10 nm) are achieved by lattice strain engineering on SrO and TiO₂ substrate terminations (self-polarisation via lattice strain) [5]. We find that the ceria termination (5nm) punctually replicates the polarisation at the BTO interface via a dynamic reconfiguration of its intrinsic defects, i.e. Ce³⁺ and V₀^{\sim}. Our experiments in different environments suggest that the BTO/ceria ferroionic design is built with a permanent polarisation that the high external fields cannot switch without the presence of polarisable media. Therefore, adding a water dielectric layer via sorption triggers different permanent polarities depending on the BTO features. These effects lead to opposite chemical states at the ceria layer, which are punctually replicated by the adsorbed water layers. The inversion of the surface potential leads to a modulation of the water adsorption-desorption equilibrium and water ionisation redox overpotentials within \pm 700 mV at room temperature, depending on the polarity of the ceria termination's charges. Overall, the results open up a possibility for tuning the catalytic properties of ceria thin films by ferroelectric engineering.

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Whispering-Gallery Mode Optoplasmonic Microcavities: From Advanced Single-Molecule Sensors and Microlasers to Applications in Synthetic Biology

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Abstract

Optical microcavities, particularly Whispering-Gallery Mode (WGM) microcavities, are highly sensitive to environmental changes and are frequently used as biosensors to detect a wide range of biomolecules and nanoparticles. To detect single molecules at the most sensitive level possible, plasmonic nanorods are incorporated to enhance the evanescent fields of WGM microcavities. This advancement in optoplasmonic WGM sensors makes it possible to detect single proteins, conformational changes, and even atomic ions, providing significant contributions to single-molecule sensing. In this talk, I will discuss the exciting research prospects in optoplasmonic WGM sensing of single molecules, including the study of enzyme thermodynamics and kinetics, the sensing of single-molecule absorption via thermo-optoplasmonic sensing, emerging ultra-sensitive single-molecule sensing on WGM microlasers, and the potential applications of WGM optical microcavities in quantum sensing and synthetic biology [1,2].

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Isolating single neurons for systematic characterization of neuronal cultures

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Abstract

In the realm of stem-cell technology, the differentiation of cells into human neurons has significantly advanced in vitro translational research. Despite these advancements, there persists a level of variability within the cultures. Accurate characterization of these cultures is crucial for leveraging the research in drug discovery and the study of specific brain functions [1]. Traditional methods such as bulk RNA sequencing or immunoflu-orescence staining, while informative, can be expensive and time-consuming, lack single-cell level analysis, and fail to establish a comprehensive link between network morphology and functional aspects, particularly neural activity, and communication.

In response to these challenges, we have developed a method for the spatial and functional isolation of single neurons, enabling an in-depth exploration of their morphology. Our approach involves the design of polydimethylsiloxane (PDMS) microstructures capable of non-invasively isolating individual neurons and spatially separating axons from the soma [2]. This design facilitates the creation of arrays comprising hundreds of single cells, providing a platform for both quantitative and qualitative analysis of cell behavior.

In our experiments, we cultured human induced pluripotent stem-cell-derived (hiPSC) NGN2 neurons [3] within these single-cell PDMS microstructures, resembling human cortical neurons. Notably, we observed a remarkable variability in cell shape and behavior, ranging from bipolar neurons with two axons extending from the cell soma to instances of single axon splitting and cells exhibiting short neurite projections. An example can be seen on Figure 1. Placing these microstructures on high-density microelectrode arrays (MEAs) [4] allowed us to record extracellular activity propagating through a single axon. We observed that single isolated neurons are spontaneously active. Continuous imaging and electrophysiology recording enabled us to track cell maturation in terms of activity and axon growth. Additionally, using PDMS microstructures we created single-cell pre- and postsynaptic neuron pairs and quantified synaptic transfer probability.

Our aim is to quantify cell culture variability based on both cell morphology and neural activity parameters. We envision creating a database of different hiPSC neuronal types and determining their types solely through the analysis of cell morphology and activity by developing a machine learning tool that would recognize the distinct differences. We believe that this method holds potential for advancing both academic research and industry by enabling a comprehensive assessment and control of cell variability in culture. Furthermore, culturing healthy and diseased hiPSC neurons as isolated single cells enables their systematic comparison in different stages of cell maturation. Combined with precision liquid handling, this approach could support in vitro pharmacological testing, as a high-throughput solution for drug discovery and development.

From Solid-State to Biophysics XI Dubrovnik (Croatia), 8-15 June 2024



Figure 1: Single NGN2 neurons or neuronal pairs isolated in the PDMS microstructures. Zoom in reveals variety of morphology within a monoculture.

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Molecular design and practical applications of nanoporous graphene membrane

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Abstract

The development of artificial structures that mimic biological channels, exhibiting superior selectivity and permeability for ions, water molecules, and gases, holds immense significance in membrane separation fields such as gas purification, water treatment, and energy conversion. Graphene, a two-dimensional material composed of carbon atoms, exhibits significant potential to serve as a novel generation of separation membrane materials, owing to its atomic thickness and ability to be perforated controllably. Moreover, its exceptional mechanical strength and chemical stability endow it with remarkable performance in extreme environments, thereby showing promising prospect in high-end applications such as aerospace and biomedicine.

Controlled introduction of nanopores plays a crucial role in separation performance. Based on this, our group focus on the molecular design of graphene nanopores and explore their potential applications. Considering the etching kinetics of graphene nanopore at the molecular level, a topdown decoupling plasma etching process is proposed to fabricate graphene nanopores with a narrow size distribution and high density, which demonstrates broad compatibility for gas phase separation, gas-liquid separation, ion screening, and dialysis processes. Then, we focus on the molecular interactions between ions and pore rim, and propose a N-doped strategy, a covalently functionalization method, and a pre-anchoring enabled directional modification method to enhance the proton transport, monovalent ions selectivity, and cation/cation selectivity, respectively. With the above methods, graphene nanopore has emerged as a promising platform for sensing with high resolution. We investigate the non-negligible effect of low-frequency on signal-to-noise ratio and achieve its control within up to 3 orders of magnitude. Furthermore, we successfully bridge the gap between laboratory-scale demonstration and commercialization to effectively utilize graphene membranes in specific applications, with an emphasis on membranebased precision instruments and membrane modules. Our findings show great potential in finetuning nanofluidic transport through molecular design of graphene nanopores, thereby facilitating the practical applications of nanoporous graphene membranes.

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Nanopore-based and waveguide-based readout of biomolecules

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Abstract

RNA modifications are ubiquitous in virtually all coding and non-coding RNA molecules, yet methods to detect them are quite demanding in terms of input requirements and further, sensitivity to modifications is limited. I will present a new approach that our group has taken to enable low-input high sensitivity RNA sequencing with sensitivity to modifications. We have recently developed electro-optical zero-mode waveguides (eZMWs) for electrically capturing picogram-level amounts of DNA and RNA linked to replicating enzymes, which is followed by real-time sequencing by monitoring the enzyme activity using high-sensitivity fluorescence inside the waveguides. We are currently integrating our approach for direct RNA sequencing by immobilizing a reverse transcriptase inside eZMWs and observing its activity using a dedicated set of fluorescent nucleotides, which will report on the RNA sequence and incorporation kinetics. Knowledge of these parameters can inform us of presence and identity of modifications in the RNA molecules.

I will also discuss our efforts to increase the throughput of protein fingerprinting using biological pores. We have recently demonstrated the use of sticky ions for generating electroosmotic flow in protein nanopores, which our group utilized for pulling unfolded proteins through nanopores. The electrical current blockade of a peptide or protein threading through a nanopore can be used as a fingerprint of the molecule in biosensor applications. After demonstrating that the combination of a chemically resistant biological nanopore, α -hemolysin (narrowest part is ~1.4 nm in diameter), and a high concentration guanidinium chloride buffer enables unidirectional, single-file protein transport propelled by an electroosmotic effect, we have begun to develop multi-channel devices that can increase throughput while preserving the required high bandwidth for obtaining protein signatures

The role of DEAD-box ATPases in the regulation of biomolecular condensates

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Abstract

DEAD-box ATPase proteins are found in all clades of life and have been associated with a diverse array of RNA-processing reactions in eukaryotes, bacteria and archaea. Their highly conserved core enables them to bind RNA, often in an ATP-dependent manner. Harnessing the energy of ATP hydrolysis, they can undergo conformational rearrangements, which enables them to unwind short RNA duplexes or remodel RNA-protein complexes. Thus, they can function as RNA helicases or chaperones. However, when their conformation is locked, they can also clamp RNA and create ATP-dependent platforms for the formation of higher-order ribonucleoprotein complexes. Recently, it was shown that DEAD-box ATPases regulate the condensation of RNA-protein complexes in vitro and control the dynamics of RNA-containing membraneless organelles in both pro- and eukaryotic cells. We will discuss how the DEAD-box ATPase DDX6/Dhh1 regulates P-bodies and how these cytoplasmic condensates function in the post-transcriptional regulation of gene expression.

Spatiotemporal Super-Resolution in Biological Systems

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Abstract

The full knowledge of a biological system requires not only information on its spatial structure but also its temporal dynamics at the highest possible resolution [1]. Spatial superresolution fluorescence microscopy has been heavily developed over almost three decades with many robust techniques now available providing localization precision well beyond the diffraction limit down to the nm scale. Temporal resolution approaches have also seen new developments, although at a slower rate. We are working with imaging fluorescence correlation spectroscopy (imaging FCS) that analyses fluorescence fluctuations at all pixels in an image to extract molecular dynamics information with at least millisecond time resolution. However, the combination of both, super-spatial and temporal resolution poses several problems. First, spatial and temporal resolution require different measurement strategies. To record dynamics, one needs the shortest possible measurement time and large pixels to preserve a sufficient signal-to-noise ratio. High spatial resolution on the other hand requires small pixels sizes and thus longer integration times. Second, the acquisition modes for spatial super-resolution are mostly customized and are not amenable to combination with fast acquisition of dynamics. Finally, the amount of data acquired requires new analytical strategies to allow data evaluation in real-time.

With the advancement in camera technology, we solve the first issue and record images at 1,000 frames per second or faster at pixel resolution smaller than 100 nm. We then bin the pixels in time to achieve spatial super-resolution, or in space for temporal super-resolution. The second issue we address by relying on computational super-resolution techniques that do not require customized microscopy methods and can be easily combined with fast acquisition modes. Using these approaches, we obtain spatiotemporal resolution with milliseconds at scales less than 100 nm. Finally, we have developed convolutional neural networks that can quantitatively evaluate the dynamics measurements in seconds, increasing evaluation speed by orders of magnitude [2].

In this seminar, we will discuss which computational super-resolution approaches are best suited for the combination with imaging FCS and how the combination of these approaches with AI creates new imaging modalities that provide spatial and temporal information on molecular processes with unprecedented resolution in real-time and at a repetition rate of seconds.

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Nanoimpact electrochemistry for biosensing

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Abstract

Stochastic nanoimpact electrochemistry is a method wherein individual nanoparticles in solution are monitored as they collide with an electrode, detected by spikes in the current-time trace. This approach enables 'digital' sensing, identifying the presence of an analyte through a distinct signal. The analyte concentration is inferred by counting the observed spikes within a specified timeframe, considering relevant mass transport mechanisms. These digital sensors possess several promising attributes for environmental or biosensing tasks. Notably, the sensing reliability scales with the number of recorded spikes and is enhanced by prolonged measurement periods or parallel recordings from electrode arrays. Introducing strategies to enhance mass transport, such as lateral flow systems, allows for rapid sensing [1]. Here, we show nanoimpactbased biosensing strategies via the oxidation of silver nanoparticles (AgNPs) at a microelectrode array (MEA). For instance, coupling nanoimpact electrochemistry with CRISPR/Cas systems enables the detection and quantification of nucleic acids, relying on the non-specific collateral cleavage activity upon target recognition. We present a proof-of-concept nanoparticle-based CRISPR/Cas-powered biosensor for selective nucleic acid quantification, illustrated in Figure 1. A readout with a high signal-to-noise ratio is achieved through single-impact electrochemical detection following nanoparticle release.

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Figure 2: Digital CRISPR-powered sensor concept. 1) A biological sample is applied to the platform. 2) In the presence of the target, collateral cleavage activity is initiated, and immobilized AgNPs are released. 3) Detection of collision events on a biased microelectrode.

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Defining shapes of crystals with undefinable surface energies

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Abstract

The equilibrium shape of crystals is a fundamental property of both aesthetic appeal and practical importance: the shape and its facets control the catalytic, light-emitting, sensing, magnetic and plasmonic behaviors. It is also a visible *macro*-manifestation of the underlying *atomic-scale* forces and chemical makeup, most conspicuous in two-dimensional (2D) materials of keen current interest. If the crystal surface/edge energy $\varepsilon(a)$ is known for different directions (angles a), its shape can be obtained by the geometric Wulff construction, a tenet of crystal physics. However, if symmetry is lacking, the crystal edge energy (or surface energy in 3D case) cannot be defined or calculated and thus its shape becomes elusive, presenting an insurmountable problem for theory. I will discuss how one can proceed with auxiliary (arbitrary or even "fake" so to speak) edge energies towards a constructive prediction, through well-planned computations, of a unique crystal shape (Figure 1). The method will be illustrated by successful shape-prediction for challenging actual materials such as SnSe which is of C_{2v} symmetry, and even AgNO₂ of C_1 , which has no symmetry at all...



Figure 1. Druses of potassium dichromate. Image by B. M. Lobastov, 2015, Wikimedia Commons.

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Label-free techniques for probing the nucleation and assembly of biomolecular condensates

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Abstract

Biomolecular condensates play important roles in fundamental biological processes such as cellular compartmentalization and regulation of biochemical processes. However, probing biomolecular condensates are challenging due to the huge span of length scales, concentration and time that their behaviour exhibits. In our recent review, we broadly surveyed label-free techniques for probing biomolecular condensate and identified a strategy – mass photometry. Focusing on dhh1 condensates – condensates associated with RNA degradation and processing, we utilized label-free microscopy, particularly mass photometry to investigate the nucleation and assembly process of dhh1 condensates. Our research aims to elucidate the role of RNA in condensate formation and its impact on protein oligomerization dynamics. Remarkably our findings unveil a new unrecognised mechanism in which the formation of these condensates is preceded by the emergence of nanodomains, suggesting a novel pathway of condensate assembly. We hypothesize that these nanodomains coalesce over time to form macroscopic condensates rather than through the conventional pathway of growth whereby the proteins are sequestered into the condensate from the aqueous phase. These findings contribute to a comprehensive understanding of the nucleation and growth process of dhh1 condensates from the single molecule to micro-scale, shedding light on the physical principles underlying biomolecular condensation at the single molecule level.



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Surface-driven Transport in 2D Nanopores

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Abstract

Streaming current, a method for converting mechanical energy gradients into electrical currents within liquid-filled environments, is investigated within the confines of ultrathin 2D WS₂ nanopores. Our studies focus on nanopores with diameters smaller than 10 nm, where we observed unexpectedly high streaming currents compared to conductive currents. Through systematic experimentation involving variations in nanopore sizes, pH, and salt concentrations, we deciphered the underlying mechanisms governing the coupling of streaming currents. Subsequently, we developed a finite element model of Poisson-Nernst-Planck and Navier-Stokes equations that incorporates modified boundary conditions at the interface between WS₂ and water. This boundary accounts for a sliding layer encompassing charge drifting in the hydrophobic layer and charge regulation dynamics. By implementing these modifications, we successfully elucidated the streaming current phenomena in nanopores of decreasing diameters, while maintaining the validity of continuum dynamics calculations. Furthermore, our model suggests a reduced surface charge requirement for generating streaming currents compared to fully mechanical boundary conditions of no slip or slip.

Distinguishing Post-translational Modifications (PTMs) along single peptides with Nanopores

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Abstract

Post-translational modifications (PTMs) play crucial roles in regulating protein function, localization, interactions, and degradation. These covalent modifications introduce new functional groups onto amino acid side chains, affecting protein structure, activity, and binding properties. Dysregulation or aberrant PTMs have been implicated in various diseases, making their precise detection and characterization critical for understanding cellular processes and disease mechanisms. While mass spectrometry remains the gold standard for protein analysis, it faces challenges in sensitivity, throughput, and sample requirements, particularly for low-abundance PTMs and complex biological matrices. Moreover, identifying the correct positions of PTMs within a protein segment is often challenging.

In our recent works, we developed a novel approach for detecting PTMs at the singlemolecule level by translocating peptides through a biological nanopore, MspA. The peptides are ratcheted up slowly by a Hel308 enzyme walking along a single-stranded DNA that is conjugated to the peptide. This controlled translocation enables the precise identification of PTM positions along the peptide sequence. Notably, we distinguished sulfation and phosphorylation on a peptide with high accuracy, even though these two modifications have similar masses and are located at closely spaced sites, separated by only one or two amino acids. This method guarantees a reliable and reproducible strategy to identify various protein PTMs, providing a new solution to many fundamental challenges in protein sequencing. By overcoming the limitations of conventional techniques, this method holds great promise for comprehensive PTM profiling, potentially leading to the discovery of novel PTM-based biomarkers and therapeutic targets. Furthermore, it paves the way for a deeper understanding of the intricate roles of PTMs in health and disease.

Sequencing by rectifying nanogaps

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Abstract

Here in this talk, we propose the simultaneous measurement of rectification and amplitude of tunneling current during electrical probing of a molecule in a nanogap for efficient singlemolecule detection. Also, we suggest the application of nitrogen-terminated graphene or CNT nanogaps due to their inherent outstanding features.

Applying DFT and Non-Equilibrium Green's Function formalism, we show that tunneling current through various molecules, including ssDNA, TATP, or small organics placed in those nanogaps, exhibits unique rectification behavior under square pulses of alternating bias. The rectification arises by on-off switching of electronic transport through the molecular HOMO or LUMO levels, sustained by partial charging of the probed molecule, generated by asymmetric hybridization of that level with Bloch states from one of the electrodes. An effect that mimics local gating, i. e. an interaction between the molecule and the nitrogen-induced dipole moment located at the N-C interface of the electrode ends, strongly influences the rectification. The simultaneous measurement of rectification and amplitude of tunneling current could be applied to gas-phase single-molecule detection, as shown in the example case of the TATP. The TATP (triacetone triperoxide) is a volatile, potent, and hard-to-detect explosive made from commonly available chemicals, a terrorist weapon of choice in the last two decades. The rectification could also be applied in the liquid phase, offering the possibility of high-throughput and precise DNA sequencing. We found that the environment (neighboring nucleotides, water molecules, and counterions) does not mask ssDNA rectification while ssDNA traverses the nanogap.

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Spin-Charge-Photon Conversion: From THz Spin-Light Coupling to Electrical Helicity Reversal

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Abstract

In solid-state systems spin-orbit coupling (SOC) is a friend and foe [1]. While SOC is responsible for the loss of information and spin depolarization, it is also crucial for transferring spin between different systems [2]. We focus on two SOC manifestations. (i) Electric dipole spin resonance in proximitized Dirac material where we reveal an overlooked resonant spin-pseudospin coupling responsible for a huge increase of THz absorption, explained by coupled spin-pseudospin torques [3], (ii) Spin-orbit torque magnetization switching, which allows to electrically reverse the helicity of the emitted light from III-V quantum dots at 300 K and zero applied magnetic field (4). We discuss the implications of these findings, from elucidating hidden proximity effects to establishing a missing link between photonics, electronics, and spintronics [5-7].

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