CMP

26 - 30 June 2023
Belgrade, Serbia

21. СИМПОЗИЈУМ ФИЗИКЕ КОНДЕНЗОВАНЕ МАТЕРИЈЕ

THE 21st SYMPOSIUM ON CONDENSED MATTER PHYSICS

BOOK OF ABSTRACTS

Institute of Physics Belgrade
Vinca Institute of Nuclear Sciences
University of Belgrade, Faculty of Physics
Serbian Academy of Sciences and Arts
Ministry of Science, Technological Development and Innovation

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21. SIMPOZIJUM FIZIKE KONDENZOVANE MATERIJE
THE 21st SYMPOSIUM ON CONDENSED MATTER PHYSICS

Conference presentations cover full range of research topics within the experimental, theoretical and computational condensed matter physics, including but not limited to the following:

S1. Semiconductor physics. Electronic structure, Quantum dots and wires, Photonic crystals, High magnetic fields phenomena, Ultra-fast phenomena.

S2. Surface, interface and low-dimensional physics. Graphene, Carbon and other nanotubes, Topological insulators, Complex oxide interfaces, Transport in nanostructures.

S3. Magnetism. Magnetic materials and phase transitions, Magneto-electronics and spintronics, Magnetic nanoparticles.

S4. Superconductivity. Conventional, high *T*c, and heavy-fermion superconductors: Materials and mechanisms, Heterostructures: Proximity effect and transport phenomena.

S5. Strongly correlated and disordered systems. Materials with strong correlations and disorder, Dynamical properties from time-resolved experiments, Quantum fluids, Cold atoms and BEC.

S6. Phase transitions, phase ordering and structural ordering of condensed matter. Equilibrium and dynamic phenomena, Ferroelectricity, Multiferroics, Quasi-Crystals, Crystal surface morphology and dynamics, Crystal growth.

S7. Soft and biological matter. Polymers, Liquids and gels, Liquid crystals, Elastomers, Membranes, Living cells and living matter.

S8. Statistical physics of complex systems. Networks and other structures.

Conference venue:
Serbian Academy of Sciences and Arts, Knez Mihailova 35, Belgrade

Conference website: www.sfkm2023.ipb.ac.rs

21. СИМПОЗИЈУМ ФИЗИКЕ КОНДЕНЗОВАНЕ МАТЕРИЈЕ

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Ministry of Science, Technological Development and Innovation

The 21th Symposium on Condensed Matter Physics - SFKM 2023, Belgrade - Serbia

Location: Main Lecture Hall -SASA Building
Kneza Mihaila 35/II Belgrade, Serbia

Date: 26th-30th June 2023

Day 1 – 26th June 2023

9:00 — 9:15	Conference opening	
Chair	***Zorica Konstantinović***	
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09:45 — 10:15	Spin injection and spin-charge conversion processes in all-oxide heterostructures	B. Martinez
10:15 — 10:45	What is quantum spin torque: Spintronics meets nonequilibrium strongly correlated and long-range entangled quantum matter	B. Nikolić
10:45 – 11:00	Proximity Induced Spin-Orbit Coupling In Phosphorene/WSe2 and WSe2/Phosphorene/WSe2 van der Waals heterostructures	M. Milivojević
11:00 — 11:20	Coffee break	

Chair	***Zoran Popović***	
11:20 — 11:50	Transport in the emergent Bose liquid: Bad metal, strange metal, and weak insulator, all in one system	W. Ku
11:50 – 12:20	Spontaneous superconducting vortex induced by stray field of skyrmion in Chiral Magnet-Superconductor Heterostructures	X. Qiu
12:20 — 12:35	The Anisotropic Interlayer Exchange In Van Der Waals 2D Magnets	S. Stavrić
12:35 – 12:50	Charge To Spin Conversion In Graphene On 1T-TaS2 Monolayer Triggered By Charge Density Wave Proximity Effects	M. Gmitra
12:50 – 13:05	Ion-atom interaction potential dependence on the ion's charge exchange	N. Starčević
13:05 — 14:30	Lunch break	
Chair	***Jelena Pešić***	
14:30 — 15:00	The Ultrafast Thermodynamics Of Graphene And Twisted Bilayer Graphene	K.-J. Tielrooij
15:00 — 15:30	Exploring Functional Properties Of Two Dimensional Materials By Atomic Force Microscopy	B. Vasić

15:30 — 15:45	Unmovable Nodal Points and Lines in Two- Dimensional Materials: Dispersions and Positions in the Reciprocal Space	V. Damljanović
15:45 — 16:00	Solving the puzzle of magnetic 2D materials – from electronic structure to magnetic interactions	D. Šabani
16:00 — 16:30	Graphene For Physiological Parameter Sensing	M. Spasenović
16:30 – 16:50	Coffee break	
16:50 – 18:50	**Round table discussion** *Discussion will be held in the Serbian language*	

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Chair	***Darko Tanasković***

9:00 — 9:30	Many-body localization: wanted dead or alive - from random to quasiperiodic systems	P. Prelovšek
9:30 — 10:00	Nonequilibrium transport and thermalization in strongly disordered 2D electron systems	D. Popović
10:00— 10:30	Dipole representation of half-filled Landau level	M. Milovanović

10:30— 10:45	Cumulant Expansion in the Holstein model: Spectral Functions and Mobility	P. Mitrić
10:45 – 11:00	Observation of many-body scarring in a Bose-Hubbard quantum simulator	A. Hudomal
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Chair	***Vladimir Dobrosavljević***	
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11:50 — 12:20	Disorder in FeSe1−xSx ($0 \leq x \leq 1$) superconducting crystals	C. Petrovic
12:20 — 12:50	Probing charge density wave phases and the Mott transition in 1T−TaS2 by Raman scattering	N. Lazarević
12:50 — 13:05	Uniaxial strain-induced changes in vibrational modes of FeSe	J. Pešić
13:05— 14:30	Lunch break	
Chair	***Cedomir Petrovic***	
14:30 — 15:00	Surprises in transition metal dichalcogenides revealed by interlayer charge transport	L. Forro

15:00 — 15:30	Superconductivity and Charge-Density-Wave in Kagome Metal CsV3Sb5 Revealed by NMR measurement	J. Luo
15:30 — 15:45	Evolution of Lattice, Spin, and Charge Properties Across FeSe1-xSx Phase Diagram	A. Milosavljević
15:45 — 16:00	Exploring superconductivity in doped mono- and bilayer borophenes	B. Šoškić
16:00 – 16:30	Raman Studies of Kagome Lattice Systems	R. Hackl
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9:15 — 9:45	On The Effects Of Finite Rate Driving On Disordered Magnetic Systems — Đ. Spasojević
9:45 — 10:00	Spin Activity Correlations in Driven Disordered Systems — D. Jovković

10:00 – 10:15	Higher-order Connectivity Patterns in the Correlation Structure of Complex Systems	S. Maletić
10:15— 10:45	Calcium-A life and death signal	M. Satarić
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12:05 — 12:35	The Evolution of Topological Magnetism in the Two-Dimensional Limit	G. Eres
12:35 — 13:05	Phyllosilicates as a platform for air-stable 2D magnetism	C. Teichert
13:05 — 13:35	Rare earth spin frustrated systems	Q. Zhang
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Chair	***Stevan Nađ-Perge***	
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9:30 — 10:00	Tuning Phases and Physical Properties of RENiO3	M. Radović
10:00— 10:30	Binary Oxides and Ferroelectricity: Ab-initio Insights Into The Polar-state Formation And Its Switching	M. Ležaić
10:30— 10:45	Analysis Of Two-Dimensional Crystals Via Rainbow Scattering	M. Hadžijojić
10:45 - 11:00	MoxWx-1S2 Nanotubes For Advanced Field Emission Application	B. Višić
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11:50 — 12:20	Spectral Functions and Mobility of the Holstein Polaron	D. Tanasković
12:20 — 12:50	Nanostructure View Of Electronic Transitions In Selected Van Der Waals Quantum Materials	E. Božin
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Chair	***Marjana Ležaić***	
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15:00 — 15:30	Effect of Large Quantum Correlations in “Russian Doll” Quantum Dots: Impact on MEG Solar Cells	S. Tomić
15:30 — 15:45	A Nonequilibrium-Thermodynamics Perspective on Charge Separation in Organic Solar Cells	V. Janković
15:45— 16:00	Soft Cluster Crystals in Simulation and Experiment	N.Adžić
16:00— 16:30	How Can We Benefit From The Optical Properties Of Mn5+ To Make Pigments And Near-Infrared Phosphors?	M. Dramićanin
16:30 — 16:50	Coffee break	
Chair	***Stanko Tomić***	
16:50 — 17:20	Fabrication of hybrid Janus particles and their application as light-driven micromotors	V. Djoković
17:20 – 17:50	Designing of a “perfect” porphyrin molecule for the Mechanically Controllable Break Junction Experiments	D. Dulić

17:50 — 18:05	Single-Molecule Probing By Rectification in a Nanogap	R. Žikić
18:05 – 18:35	Collective dynamics of social systems: a statistical physics approach	M. Mitrović Dankulov

Day 5 – 30th June 2023

Chair	***Dragana Popović***	
9:00 — 9:30	TBA	M. Drndić
9:30 — 10:00	Efficient Photon and Phonon Interfaces for Spin Qubits in Diamond	M. Lončar
10:00— 10:30	Stability of vortices in dipolar droplets	A. Balaž
10:30— 11:00	On the Theoretical Description of Photon Bose-Einstein Condensates	A. Pelster
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Special session: Celebrating Milan Damnjanović's 70th Birthday Jubilee

Chair	***Časlav Brukner***	
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12:00 — 12:30	Superconductivity, Topology and Correlations In Twisted And Untwisted Graphene Structures	S. Nadj-Perge
12:30 — 13:00	Excitons and phonons in van-der-Waals 2D materials	J. Maultzsch
13:00 — 13:30	Finding Useful Metastable Materials – New Perspectives on an Old Problem	V. Stevanović
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Chair	***Janina Maultzsch***	
14:30 - 15:00	Crystal Closed Shell	M. Damnjanović
15:00 – 15:30	Quantum Reference Frames: what they are and what they're good for	Č. Brukner
15:30 - 16:00	Reconstruction of Quantum Particle Statistics: Fermions, Bosons and Beyond	B. Dakić
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INVITED TALKS

Stability of vortices in dipolar droplets

Milan Radonjić[a,b], Axel Pelster[c] and Antun Balaž[a]

[a]*Center for the Study of Complex Systems, Institute of Physics Belgrade, University of Belgrade, Serbia*
[b]*I. Institute of Theoretical Physics, University of Hamburg, Germany*
[c]*Physics Department and Research Center OPTIMAS, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Germany*

Abstract. Vortices in dipolar Bose-Einstein condensates have been studied theoretically and numerically for a long time, but have proved to be elusive and were experimentally observed only very recently [1]. Based on variational calculations, it was suggested [2] that vortices may also exist in dipolar droplets [3], exotic quantum states that emerge due to quantum fluctuations [4]. Here we study if self-bound dipolar droplets can support vortices using numerical approach based on the extended Gross-Pitaevskii equation, which includes quantum depletion and finite-size corrections. We also study dynamical stability of such vortex states for experimentally relevant values of system parameters.

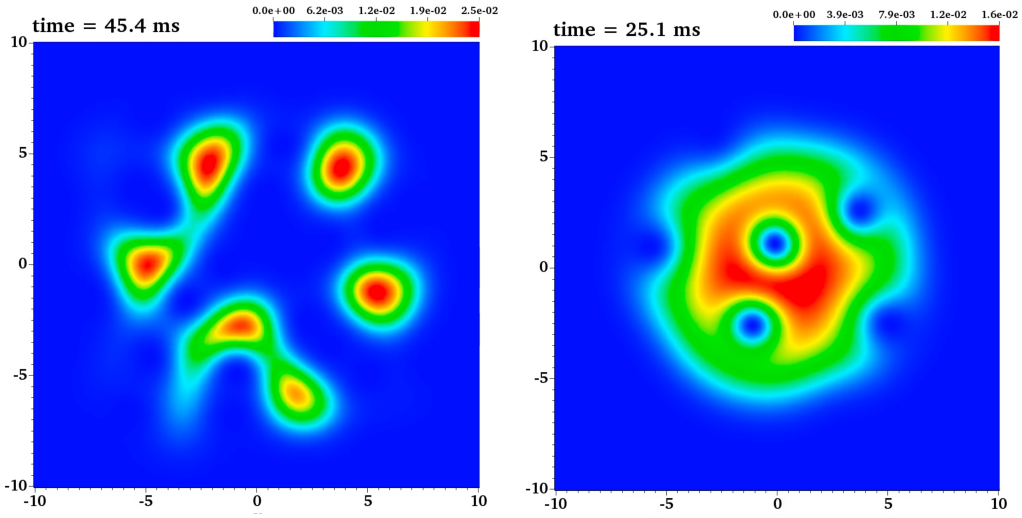

FIGURE 1. Quantum droplets and vortices in a rotating dipolar Bose-Einstein condensate of ^{164}Dy.

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Nanostructure View Of Electronic Transitions In Selected Van Der Waals Quantum Materials

Emil S. Bozin

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Abstract. Layered structural architectures, such as van der Waals transition metal dichalcogenides and related materials, host diverse phenomena including charge density waves, superconductivity, quantum spin liquid and topological phases, offering a fertile platform for exploring interplay of electronic degrees of freedom (charge/orbital/spin), electronic phase competition and the role of effective lattice dimensionality. Here we present results of nanoscale structure mapping, based on analysis of X-ray total scattering experiment data collected at National Synchrotron Light Source II at Brookhaven National Laboratory, across well-known electronic transitions in two exemplar layered materials. In the first example, local structure analysis tracks evolution of the Star of David distortions across a cascade of charge density wave transitions and the purported quantum spin liquid state in a prototype layered dichalcogenide Mott insulator 1T-TaS_2. This reveals appearance of locally broken symmetry state at temperatures well above the appearance of long-range order, implying that charge ordering is driven by polaron crystallization into a Wigner crystal-like state, rather than Fermi surface nesting or conventional electron-phonon coupling. The analysis unveils a new symmetry-restoring transition into an interlayer dimerized state near 50 K and demonstrates, via in situ 1T-to-6R polytype transformation at high temperature, that the polarons are the property of 1T-type layers where Ta are octahedrally coordinated by sulfur. The second example focuses on $ZrTe_5$, a Dirac semimetal exhibiting anomalous Hall effect and chiral magnetic effect, where its centrosymmetric structural degrees of freedom have been thus far considered inert. This system also hosts a mysterious low temperature resistivity anomaly that has puzzled researchers for nearly five decades, leading to early speculations that it derives from a structure symmetry breaking phase transition or a charge density wave formation, and more recently attributed to a Lifshitz transition, a topological phase transition, or Dirac polaron formation. Temperature dependent total scattering analysis demonstrates an unambiguous link between the anomaly and nanoscale atomic structure, indicating importance of interlayer correlations (Fig. 1) and likely role of phonons, further hinting towards local inversion symmetry breaking in the temperature regime above the anomaly in $ZrTe_5$.

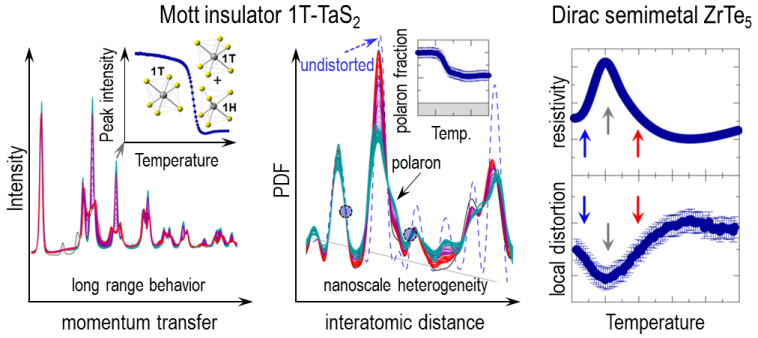

FIGURE 1. The 1T-to-6R polytype transformation in TaS_2 from the average (left) and the local (center) structure perspective. Correlation of local distortions and the resistivity anomaly in $ZrTe_5$ (right panel).

Quantum Reference Frames: what they are and what they're good for

Caslav Brukner[a]

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Abstract. When describing a physical system, it is very common to do so with respect to a reference frame - a ruler used to determine the position of a particle, for example, or a clock, which tracks the time evolution. Usually, reference frames are treated as classical objects with well-defined properties. But what happens if we take into account the quantum properties of the reference frame itself? In this talk, I will give an introduction to the basic idea and formalism of quantum reference frames, which aims to address this question. Moreover, I will explain how these generalized reference frames can be used to extend the classical symmetries of a theory to the quantum level – a research field that has been in focus of interest of Milan Damjanovic.

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2. Giacomini, F., Castro-Ruiz, E., & Brukner, Č., Relativistic quantum reference frames: the operational meaning of spin. *Physical review letters*, 123(9), 090404 (2019).
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4. Apadula, L., Castro-Ruiz, E., & Brukner, Č., Quantum Reference Frames for Lorentz Symmetry, arXiv:2212.14081 (2022).

Reconstruction of Quantum Particle Statistics: Fermions, Bosons, and Beyond

Borivoje Dakić[a]

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Abstract. Identical quantum particles exhibit only two types of statistics: bosonic and fermionic. This limitation is due to *ad hoc* assumptions added to quantum formalism, ranging from the symmetrization postulate to the underlying space topology assertions. Following the instrumentalist approach to quantum theory [1,2], in this talk, I will present a novel framework for quantum statistics, where identical particles are embedded in an operationally well-defined setup composed of laboratory primitives, such as preparations, transformation, and measurements. In such a scheme, indistinguishability is directly incorporated through measurements in which detectors can only register particle numbers but cannot distinguish them. I will derive an operational characterization of quantum particle statistics based on two simple constraints, i.e., that a) the (standard) unitary group defines single-particle transformations, and b) independent transformations act locally in the state space. The classification includes bosons and fermions, but also novel statistics appears accompanied by hidden symmetries and new degrees of freedom. These new statistics exhibit intriguing phenomena, such as the generic degeneracy of ground states and spontaneous symmetry breaking, which are absent in ordinary statistics.

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Crystal Closed Shell

Milan Damnjanović[a,b], Ivanka Milošević[b]

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[b]*NanoLab, Faculty of Physics, Studentski Trg 12, Belgrade 11000, Serbia*

Abstract. Quantum mechanical notion of closed shell, introduced for angular momentum and widely used in molecular physics, is analyzed and generalized to symmetry groups relevant for solid state physics (low-dimensional crystals, in particular). It turns out that the most natural definition of the crystal closed shell refers to the (quasi)band representations of the (connected) band structures. The well-known fact that the determinant representation of the angular momentum closed shell is the unit representation, cannot be straightforwardly generalized. In fact, the closed shell determinant representations of low-dimensional crystals groups are neatly related to topology: emergence of non-unit representations reveals stable (in the K-theoretical sense) topological bands of 2D crystals (layer group symmetry) and obstructed atomic limits of 1D crystals (line group symmetry).

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3. Milošević, I., Dmitrović, S., Vuković, T., Dimić, A. and Damnjanović, *J. Phys. A: Math. Theor.* **53**, 455204 (2020).

Mott quantum critical phase of FeO dominates Earth's lower mantle

Vladimir Dobrosavljevic

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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 the electronic structure of B1-FeO at extreme conditions with large-scale theoretical modeling using state-of-the-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 (~ 10^5 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 magnet field evolution.

How Can We Benefit From The Optical Properties Of Mn^{5+} To Make Pigments And Near-Infrared Phosphors?

Miroslav D. Dramićanin

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Abstract. When tetrahedrally coordinated in crystals, Mn^{5+} optical centers ([Ar]$3d^2$ electron configuration) always encounter a strong crystal field. Their lower electronic states have an energy progression of $^3A_2 < {}^1E < {}^1A_1 < {}^3T_2 < {}^3T_1$. The ground state ($^3A_2$) is not orbitally degenerate, and the first excited state ^1E has almost no nuclear displacement relative to the ground state and can be separated by the low-symmetry ligand field. For these reasons, Mn^{5+}-doped compounds may provide a strong and narrow (FHWM < 5 nm) phosphorescence emission in the near-infrared (1110–1300 nm) which is significantly affected by a nephelauxetic effect. Their strong absorption in the red spectral region, associated with the $^3A_2 \rightarrow {}^3T_1(^3F)$ electronic transition, provides intensive turquoise/blue coloration of the materials. Herein, we propose the way to engineer pigments and efficient near-infrared phosphors and demonstrate optical properties of several of them (Mn^{5+}-activated $Ca_6Ba(PO_4)_4O$ [1], $Sr_3(PO_4)_2$, $Ba_3(PO_4)_2$, and $Ba_3(VO_4)_2$). In addition, recent applications of these materials are highlighted, including luminescence thermometry [2] based on phosphors steady-state [1] and time-resolved [3] near-infrared emission, the latter of which has been demonstrated for biomedical applications.

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Designing of a “perfect” porphyrin molecule for the Mechanically Controllable Break Junction Experiments

Diana Dulić

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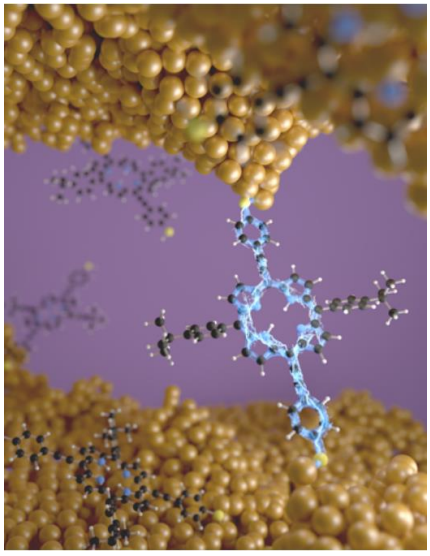
Abstract. The biggest challenge of molecular electronics is to condense the functionality of an electronic device into a single molecule and to exploit the functional versatility offered by the chemical diversity of molecules for electronic device purposes. Porphyrins and their related macrocycles are promising building blocks for the construction of bio-inspired molecular devices. Nature itself offers magnificent examples of porphyrin usefulness, such as activating and transporting molecular oxygen in mammals and harnessing sunlight in plant photosynthetic systems. In spite of their potential, obtaining well defined single-molecule conductance features is a difficult task. Due to π-stacking porphyrins can form a variety of junction configuration, leading to a large spread in conductance values using the mechanically controllable break junctions (MCBJ) technique. This limits the further progress in investigating the molecular functionalities on a single molecule level in porphyrin molecules. In this presentation, I will show that by close interaction between synthetic chemists and physicists a “perfect” porphyrin molecular design for mechanically controllable break junctions can be achieved, leading to well defined, highly conducting molecular junctions. This opens further prospects for “porphyronics” – porphyrin-based molecular electronics.



Fabrication Hybrid Janus Nanoparticles And Their Application As Light-Driven Micromotors

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Abstract. Interest in developing micro/nano motors (MNMs) increased rapidly in the last couple of years. These advanced systems can address critical challenges in manipulation of objects at small-scales. Micro/nano motors are capable to move controllably in fluids under the influence of various stimuli (thermal, magnetic, light, etc.) and perform specific operations, including propelling micromachines. Here we synthesized two types of hybrid Janus particles, Au-TiO_2 and $AgAg_2S$-TiO_2, and tested them as possible light-driven micromotors. Light, as a versatile power source, allows non-invasive control of the motion of the motors with high spatial and temporal resolutions. Illumination induce asymmetric reactions on the two sides of the Janus particles, which can create the propulsion. To optimize the properties of the MNMs, we performed synchrotron radiation gas-phase photoemission spectroscopy (SR PES) of the free standing hybrid particles at synchrotron SOLEIL, France. SR PES provided an information about the valence level alignment of the components, possible hybrid states and dominant scattering processes.

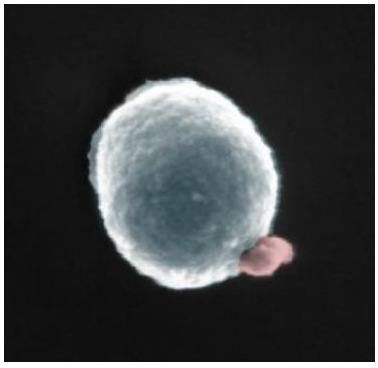

FIGURE 1. TEM micrograph of Au-TiO_2 Janus particle (size ~400 nm)

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Physics and Geometry Beyond the Limits of Uncertainty Relations

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Abstract. In the general conceptual framework of C*-algebraic physics and geometry, we describe an array of related non-commutative structures exhibiting properties interesting from both mathematical and physical perspectives. We visit 3 classes of examples:

The first and principal one is given by the *contextual subquantum theories*. Such theories satisfy a number of important consistency conditions, intrinsically related to overcoming the obstacles by the von-Neumann, Gleason and Bell no-go type of theorems, and reflecting on the underlying mathematical structure for observables and states. The whole structure is painted in terms of appropriate non-commutative C*-algebraic extensions of commutative classical-type observables for the subquantum state spaces. This, in turn, naturally suggests a holistic interpretation of physical reality, in which phenomena are not fully describable in terms of separate physical objects.

We then discuss purely geometric counterparts for these non-commutative subquantum models and their interpretations.

Finally, a charming class of examples emerges when we consider the C*-algebraic extensions naturally associated to the symmetry group of a crystal lattice and its Brillouin Zone.

The Evolution of Topological Magnetism in the Two-Dimensional Limit

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Abstract. The intrinsic magnetic topological insulator family $MnBi_2Te_4/(Bi_2Te_3)_n$ is an ideal model system for exploring exotic phases of matter including the quantum anomalous Hall insulator, the axion insulator, and Weyl fermions. Ideally, the properties of these self-organized superlattices are governed by the sequence of ferromagnetic $MnBi_2Te_4$ septuple layers (SL), and non-magnetic Bi_2Te_3 quintuple layers (QL). In contrast to bulk crystals, thin film growth by molecular beam epitaxy (MBE) provides extra tuning parameters for controlling the composition and the layer sequencing to create desired magnetic topological states. Here, we explore the electronic and magnetic response as a function of chemical composition, layer stacking and surface termination in heterostructures grown by MBE. These data reveal a delicate dependence of the overall magnetic and electronic response of $MnBi_2Te_4$ on the stoichiometry of individual layers. Specifically, we observe a dramatic reversal of the sign of the anomalous Hall effect driven by finite thickness magnetism, which suggests that the films split into distinct magnetic layers each with a unique electronic signature. This behavior is attributed to changes of intralayer ferromagnetic and interlayer antiferromagnetic exchange coupling governed by compositional and structural perturbations. Air exposure of compositionally optimized high quality thin films creates additional perturbation that results in inadvertent environmental doping. We used neutron reflectivity measurements to show that surface oxidation is confined to the top 1-2 unit cells. Our study concludes: 1) that perturbations resulting from oxidation used during MBE growth or in post growth processing of both thin films and exfoliated bulk crystals may play an important role in stabilizing the quantum anomalous Hall effect in this system, for example by tuning the Fermi level, and 2) that MBE combined with targeted modifications to the surface composition opens new avenues for engineering novel topological and magnetic phases in this fascinating material.

Research sponsored by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Sciences and Engineering Division.

Spin phenomena in van der Waals heterostructures

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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]. In addition, graphene with strong proximity spin interactions can host novel topological states [2]. Fascinating new phenomena appear when bilayer graphene gets encapsulated by a TMDC from one side, and a ferromagnet from another. The resulting, so called ex-so-tic structure [3], offers spin swap functionality: switching spin-orbit and exchange coupling on demand by gate. In this talk I will review the recent developments in the proximity phenomena in graphene, and present some recent theoretical results on the control of the proximity spin-orbit and exchange coupling by twisting the van der Waals layers. I will show that the signature proximity spin-orbit coupling in graphene---valley Zeeman coupling---can be efficiently tuned by the twist angle [4], and that proximity exchange coupling can be switched by the twist angle, and even morph from ferromagnetic to antiferromagnetic [5]. Support from DFG SPP1244, SFB 1277, FLAGERA 2DSOTECH, and EU Graphene Flagship is acknowledged

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Surprises in transition metal dichalcogenides revealed by interlayer charge transport

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Abstract. The ascending strategy for functionalizing layered Van der Waals materials is the manipulation of the coupling between atomic sheets to create novel tunable electronic states with exploitable properties. The responsible interactions can be sensitively tested by the interlayer charge transport, which has remained largely unexplored due to associated experimental challenges. By employing focused ion beam (FIB) microfabrication we accomplished a detailed study of the resistivity anisotropy in monocrystalline, bulk Transition Metal Dichalcogenides (TMDs) — like 1T-TaS2 and 2H-NbS2. These measurements have revealed number of surprises, which will be reported.

Acknowledgment. Edoardo Martino, Konstantin Semeniuk and Helmuth Berger are acknowledged for their key contributions.

Raman Studies of Kagome Lattice Systems

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Abstract. Materials with atoms occupying sites on a kagome plane attracted increasing attention after the discovery of AV_3Sb_5 systems (A = K, Rb, Cs) exhibiting charge order and superconductivity. Yet, the starting point for the research into this material class was magnetism, which, in the case of antiparallel spin order such as in herbertsmithite, is frustrated due to the triangular coordination. Ferromagnetic order appears to be more straightforward to deal with since frustration is irrelevant here. However, ferromagnetism breaks time reversal symmetry and may entail topologically interesting objects such as Weyl nodes or points. Dirac points in the electronic structure emerge generically in the underlying honeycomb lattice. Thus, ferromagnetic Fe_3Sn_2 remains interesting also at low temperature in spite of the high Curie point at T_C = 670 K and, in fact, exhibits a rotation of the ferromagnetically ordered Fe spins from out of the kagome plane to in plane between 100 and 150 K. The lattice is almost ignorant of this rotation but our Raman experiment show that the lowest fully symmetric phonon senses this rotation: Below 100 K the damping of the phonon decreases rapidly indicating a contribution of the lattice to this rotation. Although vanadium is potentially magnetic in some oxidation states, CsV_3Sb_5 is nonmagnetic at all temperatures but rather displays charge order (CDW) below T_{CDW} = 94 K and superconductivity below $T_c \approx 2.7$ K. Thermodynamic studies suggest that the phase transition at T_{CDW} is first order challenging the usual weak-coupling mean-field picture. Similarly, no anomaly in the acoustic phonon branches is found, and the ordering vector changes in the 40 K range. The Raman experiments reveal a discontinuity of an optical phonon at T_{CDW} thus indicating at least intermediate coupling. In addition, two amplitude modes are identified which do not follow the mean-field prediction but rather set in at finite energy and thus also support the first-order scenario. Finally, also the huge electronic gap argues for strong coupling. Although we are not yet in a position to identify the driving mechanism for the CDW, strong-coupling effects in the electronic and lattice properties cannot be neglected.

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Time Reversal Symmetry Breaking And Bogoliubov-Fermi Sufraces In Multiband Superconductors

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Abstract. Multiband electron systems often require multicomponent superconducting order parameter, which naturally leads to time reversal symmetry breaking, in principle, accompanying the superconductivity. I will discuss how and why this combination almost inevitably leads the appearance of small surfaces of zero-energy Bogoliubov excitations, instead of the usual gap, points, and lines. In particular, I will show how the presence of inversion symmetry, previously thought to be crucial, is actually unimportant for this phenomenon

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Prediction of 1st order Phase Transition with Electron-Phonon Coupling

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Abstract. At the phase transition temperature (PTT) the Gibbs energy *G*, respectively for negligible volume change the free energy *F*, are continuous, but not analytical. PTs as a function of temperature arise to the shifting balance between the (binding) energies and the entropic contributions of the different crystal structures above and below the PTT. Generally speaking, in a solid the binding energy is mainly determined by the electronic configuration, whereas the entropic contribution arises due (low) phonon frequencies [1]. From a conceptional point of view, such an approach is not satisfactory, because the **same** ab initio- Hamiltonian describes the high as well as the low temperature phase (HTP / LTP). The different solutions for *F* and the PT arise, because temperature redistributes the eigenenergies differently.

We address this problem and model 1st order PTs by adding electron phonon interaction (EPI) to the Hamiltonian. With increasing temperature, electronic energies (fermions) are less affected than the phonon (bosons) related enhancement of entropy. Already Ginzburg [2] proposed such an approach coupling electron and lattice dynamics through electron phonon interaction and to derive through the nonanalyticity or discontinuity of the derivatives of *F* the PT. EPI has been taken up by Kristoffel and Konsel [3]; they could clearly correlate the shift of the nucleus changing from one phase to another, however, their approach only led to a 2nd order transition (continuous shift of the nucleus), because the computed *F* turned out to be once differentiable. The approximation employed by KK neglected the kinetic energy of the nucleus with the consequence of a coarse description of soft phonons and their entropic contribution. The here pursued path to calculate *F* is based on the Bogolyubov inequality [4], used to evaluate the free energy of the Hamiltonian, now including the kinetic energy operator of the nucleus. We derive an implicit equation for the critical temperature of the first-order PT, an approximative expression for the latent heat and the positional shift of the nucleus. Comparison with ref [3] allows to determine temperature boundaries for 1st and 2nd order PTs.

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Group-IV SiGeSn Alloys For Photonics and Electronics – Recent Progress

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Abstract. The target of group-IV photonics is the integration of group-IV alloy based (opto)electronic components on silicon substrate, with all the benefits coming from mature and cost-effective fabrication. The most important, but still missing component is the electrically pumped laser operating at room temperature. Lasing requires a direct bandgap, which is generally achievable by appropriate alloy composition and strain. Since the first demonstration of GeSn laser [1], which was optically pumped and operated up to 90K, but only in pulsed mode, significant research effort has been put into this area, by modifying the alloy composition (while keeping good crystal quality), applying strain to modify the band structure, and considering the low-dimensional structures instead of bulk material. By introducing tensile strain into GeSn by SiN_x stressor, which increases the directness of the GeSn alloy, optically pumped continuous-wave lasing up to 70K was achieved [2]. Recent significant advances were the demonstration of room temperature lasing in optically pumped GeSn [3], and of electrically pumped laser operating up to 90 K, using SiGeSn/GeSn/SiGeSn double heterostructure [4]. Theoretical modelling indicates that GeSn/SiGeSn QW lasers may provide even better performance [5,6], if high-quality structures growth is achieved. Another possible application of SiGeSn alloys is for thermoelectrics, and recent results indicate good prospects for TE power conversion, the figure of merit of ZT ~ 0.4 at 300 K, and an impressive 1.04 at 600 K [7] was recently achieved in bulk $Ge_{0.86}Sn_{0.14}$ [7].

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Transport in the emergent Bose liquid: Bad metal, strange metal, and weak insulator, all in one system

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Abstract. Non-saturating high-temperature resistivity ("bad metal"), *T*-linear low-temperature resistivity ("strange metal"), and a crossover to activation-free growth of the resistivity in the low-temperature limit ("weak insulator") are among the most exotic behaviors widely observed in many strongly correlated materials for decades that defy the standard Fermi liquid description of solids. Here we investigate these puzzling behaviors by computing temperature-dependent optical conductivity of an emergent Bose liquid and find that it reproduces all the unexplained features of the experiments, including a featureless continuum and a well-known mid-infrared peak. Amazingly and with physically intuitive mechanisms, the corresponding doping- and temperature-dependent resistivity displays the bad metal and strange metal simultaneously and sometimes weak insulating behaviors as well. The unification of all these non-Fermi liquid behaviors in a single model suggests that a new quantum state of matter, namely the emergent Bose liquid, will guide the development of the next generation of solid state physics.

Probing charge density wave phases and the Mott transition in 1T−TaS_2 by Raman scattering

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Abstract. We present a polarization-resolved, high-resolution inelastic light scattering study consecutive CDW regimes in 1T-TaS_2 single crystals, supported by ab initio calculations. The analysis of the spectra within the low-temperature C-CDW regime suggests $P\bar{3}$ symmetry of the system. The spectra of the high-temperature IC-CDW phase directly project the phonon density of states due to the breaking of the translational invariance, supplemented by sizable electron-phonon coupling. Between 200 and 352 K, our Raman spectra show contributions from both the IC-CDW and the C-CDW phases, indicating their coexistence in the NC-CDW phase. The temperature dependence of the symmetry-resolved Raman conductivity indicates the stepwise reduction of the density of states in the CDW phases, followed by a Mott transition within the C-CDWphase. By means of inelastic light scattering, we were able to determine the size of the Mott gap at 170–190 meV, and to track its temperature dependence.

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Binary Oxides and Ferroelectricity: *Ab-initio* Insights Into The Polar-state Formation And Its Switching

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Abstract. In ferroelectric memory cells, information can be encoded in the direction of the electric polarization of a ferroelectric material, that can be externally switched by an electric field. While the already commercialized capacitor-based ferroelectric random access memory requires a destructive read-out, novel concepts such as ferroelectric field-effect transistors, FeFETS, or ferroelectric tunnel-junctions, FTJs, overcome this deficiency and offer the possibility of improved scalability. In order to achieve the latter, however, new ferroelectric materials are needed. One that recently immerged as a promising candidate is ferroelectric hafnia, HfO_2, a material whose compatibility with CMOS technology stimulated many studies, experimental and theoretical alike [1].

Using density functional theory combined with an evolutionary algorithm, we investigated ferroelectricity of substoichiometric hafnia, $HfO_{2-\delta}$, with δ=0.25, and found a somewhat unconventional polarization switching path, bearing similarities to the ferroelectric switching we also find in thin films of multiferroic ε-Fe_2O_3 [2,3]. I will present our results, which provide a possible explanation for the experimentally observed fatigue and wake-up effects in hafnia-based ferroelectrics [4].

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Efficient Photon and Phonon Interfaces for Spin Qubits in Diamond

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Abstract. Color centers in diamond have emerged as promising quantum memories of interest for realization of quantum repeaters and quantum networks[1]. Among these, silicon-vacancy (SiV) color centers are of particular interest owing to their long spin coherence times at cryogenic temperatures and good optical properties. Furthermore, these systems have strong susceptibility to strain[2] which allows them to be controlled using acoustic modes[3]. I will present our work on optical[4] and acoustic cavities and waveguides that can be used to prepare, control and read out the quantum states of electron and nuclear spin qubits associated with SiV.

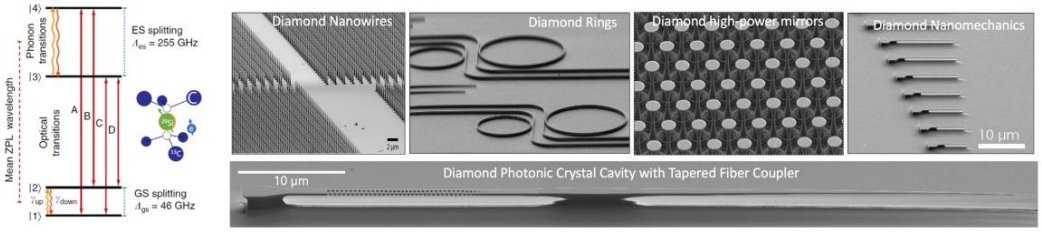

FIGURE 1. Left: Level diagram and schematic of SiV color center in diamond. Right: Optical and acoustic devices fabricated in diamond and used to enhance spin-photon and spin-phonon interactions.

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Superconductivity and Charge-Density-Wave in Kagome Metal CsV_3Sb_5 Revealed by NMR measurement

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Abstract. In this talk, we present $^{121/123}$Sb nuclear quadrupole resonance (NQR) and ^{51}V nuclear magnetic resonance (NMR) measurements on kagome metal CsV_3Sb_5 with Tc = 2.5 K. Both ^{51}V NMR spectra and $^{121/123}$Sb NQR spectra split after a charge density wave (CDW) transition, which demonstrates a commensurate CDW state. The coexistence of the high temperature phase and the CDW phase between 91 K and 94 K manifests that it is a first-order phase transition. The CDW order exhibits tri-hexagonal deformation with a lateral shift between the adjacent kagome layers, which is consistent with 2x2x2 superlattice modulation. At low temperature, electric-field-gradient fluctuations diminish and magnetic fluctuations become dominant. Superconductivity emerges in the charge order state. Knight shift decreases and $1/T_1T$ shows a Hebel–Slichter coherence peak just below Tc, indicating that CsV_3Sb_5 is an s-wave superconductor.

Spin injection and spin-charge conversion processes in all-oxide heterostructures

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Abstract. The use of the electronic spin as a control variable would allow progress in the development of high performance and low-power electronic devices compared to classic semiconductor-based devices. The development of this new technology requires strict control of the processes of generation, transmission and detection of pure spin currents. Fundamental in the generation and detection of spin currents are the spin charge interconversion processes through spin Hall effect (SHE) and inverse spin Hall effect (ISHE). In these processes the spin-orbit interaction (SOI) plays a fundamental role since it enables direct charge-spin couplingand therefore, mediates spin-charge interconversion processes whose efficiency is measured through the spin Hall angle, θSH. Therefore, potentially interesting materials for spintronics will be those having a strong SOI. Since SOI increases with the atomic number, 4d and 5d metals, such as Pt, use to have large θSH while it is usually low in 3d metals. On the other hand, there is a strong interest in the use of transition metal oxides (TMOs) since it would make it possible to exploit the great variety of functionalities that these materials possess together with a wide range of possibilities for their control and tuning. Among the TMOs, manganese perovskites are one of the most popular materials due to the wide range of functionalities they exhibit and the ease with which these functionalities can be tuned. On the other hand, iridates, which combine the possibilities of OMTs with the strong spin-orbit coupling of Ir, represent an interesting alternative as spin detectors. In this talk a study of spin injection and spin-charge conversion processes in TMOs will be presented. Ferromagnetic resonance (FMR) technique will be used to generate pure spin currents by spin pumping (SP) in ferromagnetic (FM) TMOs materials, such as La2/3Sr1/3MnO3 (LSMO), and the detection of these pure spin currents will be acomplished by measuring the ISHE transversal voltage signal in FM/normal metal (NM) bilayers. These studies will also be performed in all-oxide heterostructures using SrIrO3 (SIO) as spin detector. The role of microstructure, interfacial features and SIO layer thickness in these processes will be analyzed in LSMO/SIO heterostructures grown on top of (001)SrTiO3 substrates by RF sputtering. Microstructure of the samples and interfaces were fully characterized by advanced X-ray diffraction and High Resolution Electron Microscopy (HR-STEM).
Acknowledgements : The authors acknowledge financial support from the Spanish Ministry of Science and Innovation through Severo Ochoa (CEX2019-000917-S) and OXISOT (PID2021-128410OB-I00) and Serbian Ministry of Education, Science and Technological Development.

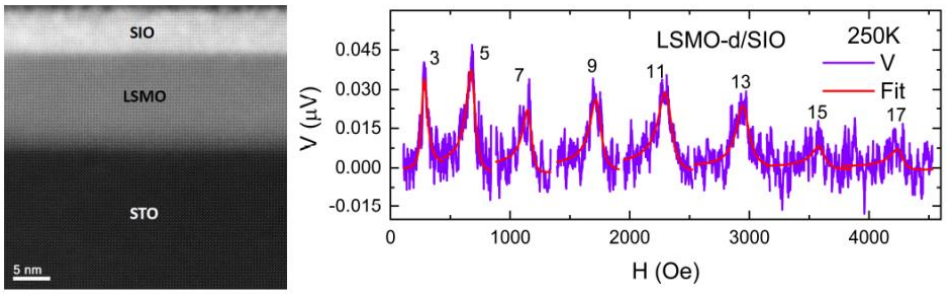

Figure 1 (left) TEM cross section of SrIrO3/La1-xSrxMnO3 heterostructure grown on SrTiO3 substrate. (right) Inverse Spin

Excitons And Phonons In Van-der-Waals 2D Materials

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Abstract. Two-dimensional (2D) materials made from layered van-der-Waals crystals have fascinating physical properties. They can be vertically stacked in almost unlimited combinations, with the twist angle between two layers as an additional degree of freedom. In this talk, recent results on optical properties of van-der-Waals stacks of semiconducting 2D materials will be presented with focus on MoS_2 and related transition-metal dichalcogenides (TMDCs). In addition, we will discuss twisted bilayers of MoS_2 and of graphene, where Raman spectroscopy can reveal the twist angle and its local variations based on resonant scattering processes. Finally, we will present antimony-based 2D materials, where the interlayer bonds have partially covalent character.

Topological States in Layered Transition Metal Dichalcogenides

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Abstract. Nowadays layered transition metal dichalcogenides (TMDs) are in focus of research as strong photoluminescent materials that could host nontrivial topological states. They appear in many crystal forms and diversity of methods of controlled structural transition are developed. For technological applications particularly interesting are the crystal phase changes which are followed by change of the band topology.

Recently, it has been shown that monoclinic 1T'-TMDs do not exhibit quantum-spin Hall (QSH) effect [1] which refutes the previous prediction of Qian et al. [2]. However, it has been shown that there are other layered monoclinic TMD structures which could host QSH state [1].

Here, analyzed is electronic band topology of a broad spectrum of mono-layered TMDs and their few-layered stacking patterns. The band structure calculation and topological characterization are performed by program POLSym [3], using topological quantum chemistry [4] and theory of symmetry indicators [5].

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From Magnonics To Neuromorphic Computing In Magnetic 2D Materials

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Abstract. Monolayer chromium-trihalides, the archetypal two-dimensional (2D) magnetic materials, are readily suggested as a promising platform for high-frequency magnonics. In this talk, I will detail the spin-wave properties of those monolayer ferromagnets, using spin-dynamics simulations parametrized from the first principles. I will show that spin-wave dispersion can be tuned in a broad range of frequencies by strain, paving the way towards flexo-magnonic applications. Further, I will reveal that the ever-present halide vacancies in these monolayers induce surprisingly strong Dzyaloshinskii–Moriya interaction, able to scatter spin-waves, which promotes design of spin-wave guides by defect engineering. Finally, I will discuss the spectra of spin-waves propagating across a moiré-periodic modulation of magnetic parameters in a van der Waals heterobilayer, and show that the nanoscale moiré periodicities in such samples are ideal for realization of a magnonic crystal in the terahertz frequency range. Recalling the additional tunability of magnetism in 2D materials by electronic gating, our results situate these systems among the front-runners for prospective high-frequency magnonic and neuromorphic applications.

Dipole representation of half-filled Landau level

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Abstract. The fractional quantum Hall effect is a phenomenon of strongly correlated electrons that is amenable to quasiparticle pictures and modeling. The presence of a strong magnetic field very often leads to the dominance of the physics inside a Landau level (LL) and it justifies approaches that assume that the description of the problem can be confined to an isolated LL. We will introduce a variant of a dipole representation for composite fermions in a half-filled LL, which takes into account the symmetry under an exchange of particles (electrons) and holes. This is implemented by a special constraint on a composite fermion and a composite hole degree of freedom (of an enlarged space), which makes the resulting composite particle (dipole) a symmetric object. We will analyze an effective Hamiltonian that commutes with the constraint on the physical space and fulfills the requirement for boost invariance on the Fermi level. The calculated Fermi liquid parameter F_2 is in good agreement with numerical investigations in K. Lee et al., which predicted Pomeranchuk instabilities in higher LLs.

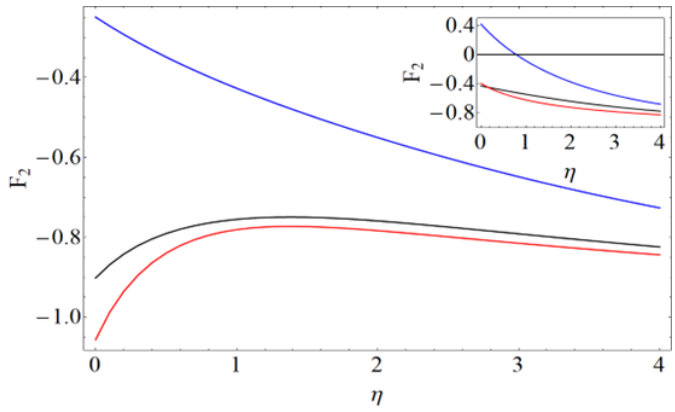

FIGURE The calculated Fermi liquid parameter F_2 for a generalized Coulomb interaction, $e^{-\eta r}/r$: the lowest LL - blue, the second LL- black, and the third LL – red. The Pomeranchuk instability is expected for $F_2 < -1$. **Inset:** F_2 with an incomplete account of the boost invariance**.** From S. Predin et al**.**

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Collective dynamics of social systems: a statistical physics approach

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Abstract. Social systems represent an important class of complex systems. They consist of a large number of interacting units and exhibit collective behavior. Phenomena that we observe in social systems, such as opinion formation, knowledge building, information, and epidemic spreading, are collective phenomena. Social systems are not static or in equilibrium. They constantly change and evolve. Statistical physics, in combination with methods from complex networks theory, sociology, and computer science, has proven adequate for studying and uncovering the fundamental principles of collective social dynamics [1]. We show different mappings of data onto a complex network and how features of these networks are related to collective dynamics, how they shape it, and how social dynamics shape them [2,3,4]. By analyzing time series of different signals from social systems, we show that this approach can be used to uncover the fundamental principles that govern social dynamics [5,4]. Using empirical analysis and theoretical modeling, we study the role of collective trust and local cohesion in sustainability knowledge-based communities [2] and the emergence of universal patterns in the growth of social groups [3]. By combining the time series with complex networks, we study the structural changes due to crises in complex systems [4]. Our results show that complex network structure influences and is influenced by the collective dynamics of these systems. Through fractal analysis of time series from different social systems, we show that self-organized criticality states co-exist with cyclical trends typically observed in social dynamics [5].

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Superconductivity, Topology and Correlations In Twisted And Untwisted Graphene Structures

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Abstract. When two graphene sheets are rotationally misaligned (i.e., twisted) by approximately one degree and stacked together, the resulting bilayer exhibits various correlated, superconducting, and topological electronic phases. The origin of these distinctive phases, emerging at this particular twist angle, can be traced back to the weakly dispersive ('flat') electronic bands in which the kinetic energy of electrons is heavily suppressed, and interactions between electrons dominate. In this talk, I will discuss several experiments providing insights into the electronic phases and band structure of twisted bilayer graphene obtained using scanning tunneling microscopy and cryogenic transport measurements. Then, I will overview several other graphene-based correlated and superconducting systems recently discovered in our lab, highlighting their striking similarities and differences. Besides bilayers, we will discuss signatures of strong correlations and unconventional superconductivity in twisted tri-, quadri-, and penta-layers and compare these findings to measurements in untwisted graphene bilayers that can exhibit similar phenomenology in strong displacement fields. Our results highlight the prevalence of superconductivity in graphene based structures.

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What is quantum spin torque: Spintronics meets nonequilibrium strongly correlated and long-range entangled quantum matter

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Abstract. The spin-transfer torque (STT), where spin-polarized current controls the magnetization of a thin layer of magnetic material, is one of the key phenomena in both basic and applied contemporary spintronics research. The "standard model" of current driven magnetization dynamics via the mechanisms of conventional (i.e., Slonczewski-Berger) spin-transfer (STT) torque is based on [2] a single-particle quantum transport treatment of flowing electrons and classical treatment of localized spins within a magnetic material via the Landau-LifshitzGilbert (LLG) equation. In the "standard model", the transfer of spin angular momentum between flowing electronic spins and localized spins occurs only if they are noncollinear. However, recent experiments [3] at low temperatures ~1 K suggest that fully quantum nonequilibrium many-body framework is required to describe situations where conventional STT is apparently zero, such as collinear but antiparallel electron and localized spins [4], or localized spins whose expectation value is zero [5] in equilibrium due to entanglement as in the case of quantum antiferromagnets, Mott insulators and quantum spin liquids. To solve this long-standing problem, we have recently [4] adapted time-dependent density matrix renormalization (tDMRG) algorithms for "quantum STT," by which we term any situation where localized spins must be treated quantum-mechanically with their individual expectation values calculated only at the end. This reveals how quantum STT can generate highly entangled nonequilibrium many-body state of all flowing and localized spins with mutual information between localized spins at the FM edges remaining nonzero even at infinite separation as the signature of dynamical buildup of long-range entanglement [4]. Another prediction from tDMRG [5] shows that interaction of spin-polarized current pulses with the surface of antiferromagnetic Mott insulator (AFMI) will transmute zero expectation value of AFMI localized spins into nonzero values. Finally, this talk provides insight into "unreasonable effectiveness" of the LLG equation in spintronics and magnonics, as well as its limitations unraveled by treating many localized quantum spins within a magnetic material in contact with a dissipative bosonic bath using quantum master equations [5], so that when the LLG modeling turns to be inapplicable the picture of "quantum STT" becomes indispensable.

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On the Theoretical Description of Photon Bose-Einstein Condensates

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Abstract. Since the advent of experiments with photon Bose-Einstein condensates in dye-filled microcavities in 2010 [1], many investigations have focused upon the emerging effective photon-photon interaction. Despite its smallness, it can be identified to stem from two physically distinct mechanisms [2]. On the one hand, a Kerr nonlinearity of the dye medium yields a photon-photon contact interaction, whose microscopic theoretical description is based on a Lindblad master equation [3]. On the other hand, a heating of the dye medium leads to an additional thermo-optic interaction, which is both delayed and non-local [4]. The latter turns out to represent the leading contribution to the effective interaction for the current 2D experiments. A new experimental platform, which is currently built up in Kaiserslautern, will be devoted to analyse the dimensional crossover in trapped photon gases from 2D to 1D. As the photon-photon interaction is generically quite weak, they behave nearly as an ideal Bose gas. Moreover, since the current experiments are conducted in a microcavity, the longitudinal motion is frozen out and the photon gas represents effectively a two-dimensional trapped gas of massive bosons, where the anisotropy of the confinement allows for a dimensional crossover. A detailed investigation for such a system allows to determine its effective dimensionality from thermodynamic quantities [5]. Furthermore, we investigate how the effective photon-photon interaction changes when the system dimension is reduced from 2D to 1D via an anisotropic harmonic trapping potential [6]. For increasing anisotropy we find that the thermo-optic interaction strength increases at first linearly with the trap aspect ratio and later on saturates at a certain value of the trap aspect ratio. In addition, we work out a Hamiltonian description of the effective photon-photon interaction that includes the thermal cloud and, thus, resembles a Hartree-Fock analogue theory for this kind of interaction [7]. Using an exact diagonalisation approach, we find that for larger trap aspect ratios the contribution of the thermal cloud can not be neglected in the analysis of experimental data.

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Disorder in $FeSe_{1-x}S_x$ ($0 \leq x \leq 1$) superconducting crystals

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Abstract. Connections among crystal chemistry, disorder and critical temperature Tc have been at the forefront of superconductivity, one of the most widely studied phenomena in physics, chemistry and materials science alike. In Fe-based superconductors Tc correlates with the average anion height above the Fe plane, i.e. with the geometry of the $FeAs_4$ or $FeCh_4$ (Ch = Te, Se, S) tetrahedron. By synthesizing $FeSe_{1-x}S_x$ ($0 \leq x \leq 1$) single crystal alloys with atomic defects we find that their Tc is not correlated with the anion height of other Fe superconductors. Instead, changes in Tc(x) and tetragonal-to-orthorombic (nematic) transition Ts(x) on cooling are correlated with Bragg plane and Fe vibrations disorder in direction orthogonal to Fe planes and thereby induced scattering rates $(1/\tau)(x)$ [1,2]. The disorder stems from deformed $Fe(Se,S)_4$ tetrahedra with different Fe-Se and Fe-S bond distances. Moreover, high-temperature metallic resistivity in the region of strong disorder exceeds Mott limit and provides an example of the strong violation of Matthiesen's rule and Mooij law which is known to be a dominant when adding moderate disorder past the Drude/Matthiassen's regime in all materials [2]. Scattering mechanism of Mott limit-exceeding resistivity is unrelated to phonons and arises for strong Se/S atom disorder in tetrahedral surrounding of Fe. Our findings shed light on the intricate connection between nanostructure details and unconventional scattering mechanism, possibly related to charge nematic or magnetic spin fluctuations.

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Nonequilibrium transport and thermalization in strongly disordered 2D electron systems

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Abstract. Understanding the dynamics of isolated disordered systems and its dependence on the range of interactions has been attracting a lot of research attention in recent years, but many questions remain open, especially in two spatial dimensions. At the same time, experiments have been limited mostly to those on synthetic quantum matter, such as ultracold atoms in optical lattices and superconducting qubits. However, observing the absence of thermalization and signatures of many-body localization (MBL) in real, solid-state materials has been a challenge.

This talk will describe experimental studies of nonequilibrium dynamics in strongly disordered, 2D electron systems with a very weak thermal coupling to the environment. We find that, while reducing the range of the Coulomb interaction has practically no effect on the dc transport, there is a striking difference in the dynamics. In the case of a long-range Coulomb interaction, the system thermalizes, although the dynamics is glassy. In contrast, in the case of a screened or dipolar Coulomb interaction, the thermalization is anomalously slow and strongly sensitive to thermal coupling to the environment, consistent with the proximity to a MBL phase. This direct observation of the MBL-like, prethermal regime in an electronic system thus 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 ensembles of interacting, disordered particles employed in previous studies of MBL. By establishing a new, versatile solid-state platform for the study of MBL, our work also opens new possibilities for further investigations, such as noise measurements as a probe of ergodicity breaking and many-body entanglement.

*This work was supported by NSF Grants Nos. DMR-1307075, DMR-1707785, DMR-2104193 and the National High Magnetic Field Laboratory (NHMFL) through the NSF Cooperative Agreements Nos. DMR-1157490, DMR-1644779, and the State of Florida.

Many – body localization: wanted dead or alive - from random to quasiperiodic systems

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Abstract. It is general observation that one-dimensional spin chains, and equivalently interacting fermionic chains, reveal a transition/crossover to the many-body localization (MBL) when subjected to large random or quasiperiodic potentials. The MBL phase should be manifested by several features as the absence of thermalization, change of spectral properties and the absence of dc transport. In spite of intensive theoretical as well as experimental efforts over last 15 years, the question of the existence of MBL and of corresponding phase transition is at present controversial. I will focus on the perspective of transport quantities [1], in particular the spin diffusion. In random systems numerical results show large sample-sample fluctuations [2], while in quasiperiodic systems this is not the case. Results for the diffusion constant reveal an exponential-like dependence on potential strength over several decades. I will present a Thouless-type relation with energy-level structure, which explains nearly linear finite-size drift of the crossover, both questioning of a well-defined MBL transition. Moreover, replacing the quasiperiodic potential with a simpler periodic one, the variation remains qualitatively similar up to large potential strengths, which offers an alternative view on the MBL problem.

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Spontaneous superconducting vortex induced by stray field of skyrmion in Chiral Magnet-Superconductor Heterostructures

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Abstract. We have designed a heterostructure of chiral magnet and superconductor in which the stray field of skyrmions can induce spontaneous superconducting vortices without applying external magnetic field. The existence of zero field skyrmions at room temperature and the subsequent spontaneous generation of superconducting vortices by the stray field of the skyrmions has been directly observed by magnetic force microscopy. The spontaneous superconducting vortices are found to locate at the center of the skyrmoins, forming skyrmoin vortex pairs with enlarged radius. The evolution of skyrmion vortex pairs with application of field has been studied.

Tuning Phases and Physical Properties of RENiO3

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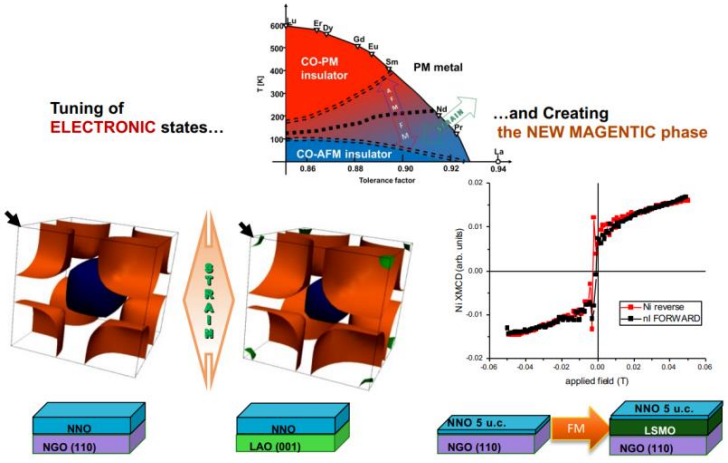
Abstract. RENiO3 (RE - Rare Earth elements) exhibit unique and multifunctional physical phenomena directly related to the spin and orbital degrees of freedom of the transition metal d-states and their interplay with the lattice. Importantly, the iso-structure of RENiO3 (RENO) permits the realization of hetero-structures altering physical matters that are very different from their bulk form. Here it will be shown through one prominent member of the RENO family, NdNiO3 (NNO), how its electronic structure and magnetic properties can be altered. Our comprehensive study establishes that substrate-induced strain tunes the crystal field splitting, consequently changing the Fermi Surface (FS) properties, nesting conditions, and spin-fluctuation strength, thereby controlling the Metal-Insulator Transition (MIT). Furthermore, the physical origin of the direct between the NNO and the magnetically ordered manganite layers in proximity will be discussed. Combined experimental methods and theoretical calculations reveal that this interaction transforms the magnetic order and electronic structure in the nickelate layer, consequently suppressing the MIT. Overall, our studies establish approaches to manipulate the properties and phases (electronic and magnetic) in NNO, signifying perspectives of TMO for novel applications.



The figure illustrates Fermi surface topology transformation via homoepitaxial strain, although the proximity to the magnetically ordered layer induces ferromagnetic ordering in NdNiO3 films. Both practices enrich the phase diagram of RENO.

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Calcium-A life and death signal

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Abstract. Almost everything that we do is controlled by calcium; how we move, how our heart beats and how our brain processes informations and stores memories. Calcium plays a key role in signal transductionin in living cells by being the chief second messenger. Calcium triggers life at fertilization and controls the developement and differentiation of cells into specific types. It tunes the subsequent activities of these cells, and finally, it is involved in cell death.

We will present our biophysical contributions clarifying the onset and the propagation of spikes of calcium signals along cellular flagella. It appears that such pulsatile increases of Ca concentrations within the cell have much higher fidelity and robustness of information transfer than simple tonic changes, since they are much less prone to noisy fluctuations. We relied on the information theories of Shannon anf Fisher in order to explain Ca signal transmission by microtubules as an optimized information pathway in flagella of sperm cells. We also will demonstrate that in the case of Ca signaling, messages difuse faster than messangers. We will explain the coding, and frequency and amplitude modulation of Ca signals, as well as, their deciphering by pertaining enzymes.

Graphene For Physiological Parameter Sensing

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Abstract. Graphene and other 2D materials represent a platform that can be used in various branches of science and technology. I will present the production of multilayer graphene by liquid exfoliation and by laser induction. Liquid exfoliated graphene is used for gas detection as well as real-time breathing detection[1]. Laser-induced graphene (LIG) is used for real-time detection of heartbeat[2] and breathing. We demonstrate sensors from these two types of graphene on various substrates, including flexible ones, showing potential for use in wearable electronics.

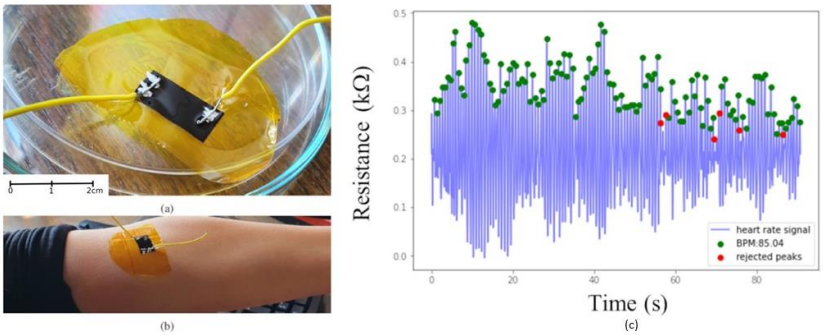

FIGURE 1. (a) Laser-induced graphene on Kapton tape. (b) LIG as heartbeat sensor. (c) Heartbeat measured with LIG sensor.

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On The Effects Of Finite Rate Driving On Disordered Magnetic Systems

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Abstract. Presented studies regarding the nonequilibrium athermal Random Field Ising model driven at finite rates reveal the existence of three driving regime types (slow, intermediate, and fast) in which the spanning events are absent/occasionally/always present. These regimes appear in 3D and 2D systems, as well as in 3D to 2D crossover, and are characterized by different shapes and scaling of the pertaining event distributions approaching adiabatic ones in the zero-rate limit. Our findings could have practical importance for the description of real systems (e.g., ferromagnetic strips and thin films) driven at constant rates, particularly those with experimental realizations that are not easily attainable.

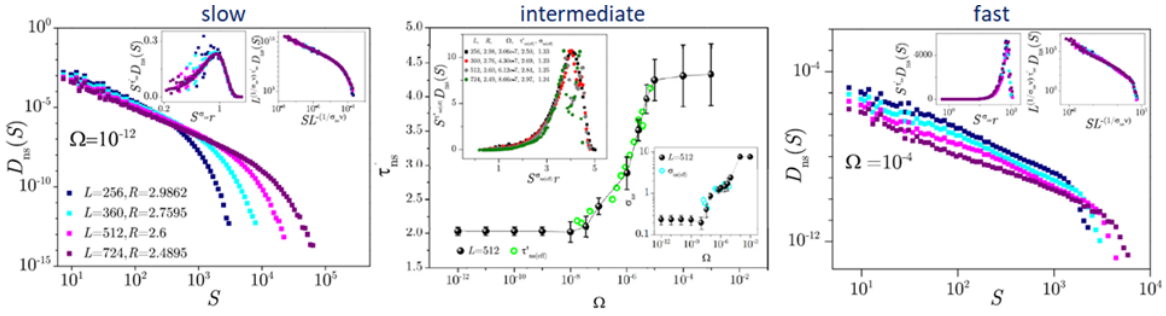

FIGURE 1. Distributions of avalanche size S in 3D model for the systems satisfying $Lr^{\nu} = const,\ \Omega r^{\nu/q} = const,\ q = 1$ The distributions are obtained in slow (left), intermediate (middle), and fast (right) regime of driving.

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Finding Useful Metastable Materials – New Perspectives on an Old Problem

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Abstract. Large-scale deployment of first-principles electronic structure calculations in combination with the ever-increasing power and availability of massively parallel supercomputers have launched in past couple of decades an entirely new paradigm in modern materials science. Intuition and serendipity that were the hallmarks of materials discovery are now complemented by theory-guided searches, which have resulted in a number of important findings. However, using theory and computations to propose, with a high degree of confidence, novel and useful metastable materials still represents a significant challenge. In this talk I will present our recent attempts to solving some of the problems hindering theory-guided discovery and design of metastable phases with the particular focus on covalent and partially ionic solids. More specifically, I will discuss experimental realizability (synthesizability) of metastable crystalline phases (or polymorphs) in connection to the specific features of the potential energy surface [1] leading to an effective computational methodology to search for, and rank potentially metastable states according to their realizability. Next, I will talk about our efforts in developing computational methods to enable large-scale assessment of the polymorph lifetimes. [2,3] These are predicated on the novel solution to the problem of finding an optimal atom-to-atom mapping between infinitely periodic systems. Lastly, an emerging description of disordered and glassy systems as statistical ensembles of ordered/crystalline local minima on the potential energy surface [4] will be discussed. This approach enables predictive modeling of atomic disorder and glasses without the need for experimental inputs. In all of these areas our recent developments offer predictions of relevant properties, which, in turn, allow for more rational and reliable searches for useful metastable materials.

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Spectral Functions and Mobility of the Holstein Polaron

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Abstract. The Holstein model is the simplest model that describes an electron that propagates through the crystal and interacts with localized optical phonons. The Holstein molecular crystal model is also very important in order to understand the role of polarons (quasiparticles formed by an electron dressed by lattice vibrations) in real materials. It remains a challenge to calculate the spectral functions and charge mobility in the whole parameter space. Here we show that the dynamical mean field theory, which becomes exact in the weak coupling and in the atomic limit, provides an excellent, numerically cheap, approximate solution for the spectral function of the Holstein model in the whole range of parameters, even in one dimension. To establish this, we make a detailed comparison with the spectral functions that we obtain using the newly developed momentum-space numerically exact hierarchical equations of motion method, which yields electronic correlation functions directly in real time. We crosscheck these conclusions with our path integral quantum Monte Carlo and exact diagonalization results, as well as with the available numerically exact results from the literature. We calculate the charge mobility in the bubble approximation and examine the role of vertex corrections.

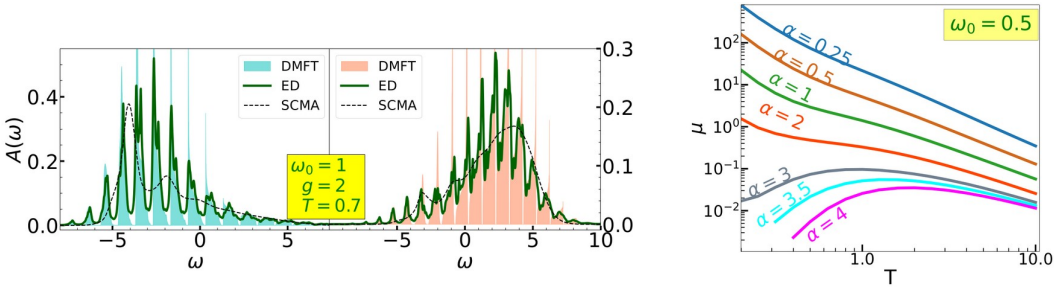

FIGURE 1. (a) Spectral functions for strong electron-phonon coupling g for k=0 and k=π. (b) Temperature dependence of charge mobility from weak to strong coupling $\alpha = g/\omega_0$.

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Phyllosilicates As A Platform For Air-stable 2D Magnetism

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Abstract. Since the first reports on intrinsically magnetic two-dimensional (2D) materials in 2017 [1,2], the price-to-pay for accessing their monolayers is the lack of ambient stability. We discovered in a mineral aggregate – mainly composed of hematite, magnetite, and chalcopyrite – soft layers of which macroscopic flakes easily could be peeled off that stuck to a permanent magnet. Employing mechanical exfoliation, we succeeded in thinning and transferring micrometer sized – mainly hexagonally shaped – flakes to SiO2 substrates. Energy dispersive x-ray spectroscopy (EDS) revealed magnesium and silica as major components of the flakes. Raman spectroscopy indicated the presence of hydroxide groups, pointing towards talc, a hydrated magnesium phyllosilicate mineral, namely talc (Mg3Si4O10(OH)2). Long-term EDS and Raman spectroscopy revealed that in the flakes about 10 % of the Mg atoms are substituted by Fe which clusters into about 20 nm regions according to scanning transmission electron microscopy. With atomic force microscopy, a minimum flake thickness of 1 nm was determined indicating cleavage down to a talc monolayer. Combined magnetic force microscopy (MFM) measurements in external out-of-plane fields up to 0.5 T and SQUID magnetometry measurements imply that the 2D Fe-rich talc exhibits weak ferromagnetic behavior [3]. The flakes are showing long-term stability under ambient conditions in contrast to the 2D magnets reported so far. Besides iron-rich talc, we investigate also ultrathin flakes of exotic minerals like minnesotaite (Mg3Si4O10(OH)2) as well as iron rich micas like biotite and annite [4]. As another approach towards iron-rich talc we propose ion implantation of iron-free talc single crystals.

Work is supported by FWF, Austria via 2020 START program (grant # Y1298 N) and has been performed in collaboration with M. Z. Khan, K.-P. Gradwohl, L. Ludescher, M. Kratzer, M. Zimmermann, R. Bakker, J. Raith (all Montanuniversität Leoben), O. E. Peil, L. Romaner (all Materials Center Leoben), C. Gammer (Erich Schmid Institute of Materials Science, Leoben), E. Fisslthaler, D. Knez, F. Hofer (Graz University of Technology), J. Genser, A. Lugstein (Vienna University Of Technology), A. Sharma, O. Selyshchev, D.R.T. Zahn, G. Salvan (TU Chemnitz), O. Selyshchev, S. Valencia, F. Kronast (all Helmholtz-Zentrum Berlin), and U. Kentsch, N. Klingner, G. Hlawacek (all Helmholtz-Zentrum Dresden-Rossendorf).

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The Ultrafast Thermodynamics Of Graphene And Twisted Bilayer Graphene

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Abstract. When light is absorbed by graphene, several interesting and technologically useful ultrafast thermodynamic phenomena occur. This typically involves electron thermalization through electron-electron interactions on a 10-100 fs timescale, followed by electron cooling by emission of phonons or by diffusion of electronic heat. In this talk, I will show two recent results related to the ultrafast thermodynamics in (twisted bilayer) graphene. The first result[1] is that the diffusion of electronic heat in graphene in the hydrodynamic regime can be exceptionally fast, as measured through spatiotemporal thermoelectric microscopy. Specifically, in the Dirac fluid regime, close to the Dirac point, we discovered a short-lived (few 100 fs) thermal conductivity that exceeds 10,000 W/m/K – even larger than the thermal conductivity of phonons. The second result[2] is that the electron cooling dynamics in twisted bilayer graphene near the magic angle is very distinct from the dynamics in monolayer or non-twisted bilayer graphene (see Figure). Specifically, the cooling time in near-magic twisted bilayer graphene is a few picoseconds all the way from room temperature down to 10 K. We ascribe this to Umklapp-assisted electron-phonon cooling, facilitated by the moiré pattern in twisted bilayer graphene.

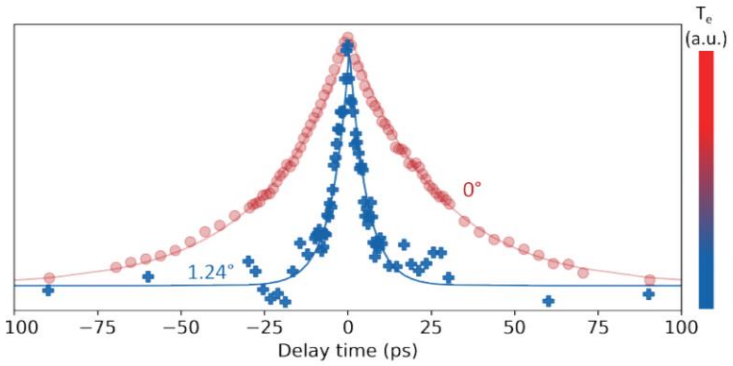

FIGURE 1. Measured electron cooling dynamics for non-twisted (red) and near-magic twisted bilayer graphene (blue) at a temperature of 25 K.

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Effect of Large Quantum Correlations in "Russian Doll" Quantum Dots: Impact on MEG Solar Cells

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Abstract. Semiconductor nanocrystals (NCs) are the subject of intensive research due to several novel properties which make them of interest for both fundamental science and technological applications. NCs are of particular interest for solar cell applications due to their ability to increase efficiency via the generation of multiexcitons from a single photon. Theoretical predictions indicate that multi-exiton generation (MEG) has the potential to enhance the efficiency of a single gap cell from 33% to 42% [1]. The efficiency of MEG in colloidal QDs is determined by the competition between MEG and other hot electron-cooling processes [2]. These have characteristic times of τ(MEG) ~ τ(cooling) ~1 ps in the colloidal QDs studied to date but for the high efficiency τ(cool) >> τ(MEG) is required. The "Russian Doll" aka core/shell QDs [3] with type II band alignment offers extra degree of freedom in mediating both the optical dipoles and the Coulomb interaction between charges in such structures. Full realization of this potential requires that the energy threshold for MEG be minimized. An attractive interaction between excitons in QD reduces the threshold by the biexciton binding energy, Bxx, but this has been found to be small (-10 meV) for type I QDs. Here, we show that, by taking into account quantum correlation effects between charges, combinations of core diameter and shell thickness can be found for a CdSe/CdTe core/shell QD that result in very large values of Bxx<0. In our analysis excitonic states were found using the full Configuration interaction (CI) method, that incudes explicitly the effects of Coulomb interaction, exact exchange and correlations between many-electron configurations in QD. In setting up the full CI, particular attention was paid to accurate modeling of the dielectric environment variation through the structure as well as surface polarization effects on core/shell and QD/colloid interfaces. Dielectric constants of constituent CdSe and CdTe around the transition energies poles are predicted using ab initio TDDFT [4]. We map the $1S^{(e)}nS^{(h)}$ (n = 1, 2) exciton correlation energy relative to the strong confinement regime as a function of core radius and shell thickness for non-uniform spatial dielectric environment [5]. We observe how the type-II confinement potentials amplifies the dielectric effect on the wave functions and exciton energies, particularly increasing the correlation energy for QDs in which the corresponding single-particle hole is delocalized [5]. We also find that correlation leads to large changes in the momentum matrix element, particularly for the lowest CdSe/CdTe QD exciton in which it is increased up to one order of magnitude in the presence of dielectric confinement. Overall dielectric confinement affected the exciton properties in CdSe/CdTe QDs more than the inverse heterostructures due to the band alignment, which encourages holes to localize in the shell. We conclude that: (i) it is not possible to predict biexciton binding using the Hartree approximation alone; it can only be predicted with a full CI Hamiltonian [6]; (ii) CI predicts Bxx = -70 meV for structures with 0.5 nm thick shell that agrees with experiment [7]; (iii) by ignoring the dielectric confinement, it is not possible to predict biexciton binding for structures with shell thickness > 0.75 nm; (iv) by changing the solvent's dielectric constant from 1 to 2 the variation in the Bxx binding energy is as

big as 100 meV; (v) a proper prediction of Bxx requires the inclusion of correlations and surface polarization effects but the effect of self-polarization is negligible. The strong biexciton binding found in Russian Doll QD is explained by the stronger reduction in the Columbic repulsion between holes than reduction in the attraction between electrons and holes upon the addition of the CdTe shell layer, Fig. 1. The Aufbau principle and Hund rule reveal this to be a consequence of 4 fold degeneracy of the hole ground state imposed by symmetry of the structure [8].

The peak efficiency in "Russian Doll" NC structures grows to 46% and then to 47% as Bxx increases to −25 and −50 meV, respectively. The largest biexciton interaction energy reported to date is ∼100 meV, although this was repulsive (i.e., antibinding) rather than attractive, it gives an indication of the magnitude of the biexciton interaction energies that can be achieved in "Russian Doll" type-II colloidal QD. For a binding energy of −100 meV, the peak efficiency rises to 50% and would rise to as much as 60% if it was possible to produce a binding of −200 meV. It can also be observed that the value of Eg corresponding to the peak efficiency shifts progressively to lower values as the photocurrent is enhanced first by MEG alone, and then by the combined effects of MEG and the onset of biexciton binding [6].

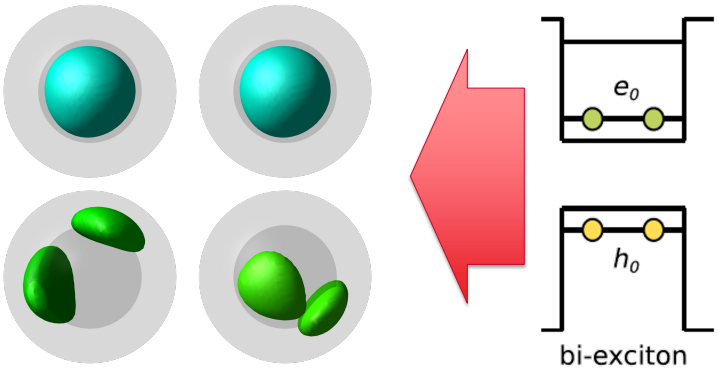

FIGURE 1. Topology of the dominant character of single particle electron/hole states in the ground state bi-exciton.

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Exploring Functional Properties Of Two Dimensional Materials By Atomic Force Microscopy

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Abstract. Two dimensional (2D) materials have a broad range of functional properties which make them appropriate candidates for various nano-electro-mechanical devices. In order to relate their mechanical, electrical, and optoelectrical properties with the local structure and morphology, microscopic techniques are prerequisite. For this purpose, we have used various methods of atomic force microscopy (AFM) which provide imaging of both morphology and physical properties with the nanoscale resolution.

The focus of the first part of the presentation is on 2D transition metal dichalcogenides, the family of 2D semiconductors with a narrow electronic bandgap and strong light-matter interaction which provide very efficient photodetection. Here we discuss photoconductive properties of WS_2 and MoS_2 and present the measurements of local dark and photo-currents using photo-conductive AFM [1]. Three different measurement methods are considered: current-voltage (I/V) characteristics, temporal response (current versus time) and 2D current maps.

In the second part we introduce novel 2D dielectrics, talc ($Mg_3Si_4O_{10}(OH)_2$) and pyrophyllite ($Al_2Si_4O_{10}(OH)_2$), obtained from naturally occurring and abundant van der Waals minerals belonging to the group of phyllosilicates (sheet silicates or clays). First we discuss the local current measurements done by conductive AFM which reveal that 2D pyrophyllite flakes behave as efficient electrical insulators with a breakdown voltage of around 6 MV/cm [2]. Therefore, these materials could be used as van der Waals dielectrics in 2D heterostructures and potentially replace standard hBN. At the same time, layered structure of 2D phyllosilicates provides easy shearing between constituent layers, the property necessary for a good lubrication. Here we present the results of the nanoscale measurements done by friction force microscopy [2, 3]. They show that 2D talc and pyrophyllite flakes exhibit a low friction coefficient of around 0.1 which makes them suitable candidates for low-cost solid lubricants in nano- and micro-mechanical devices.

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Rare-earth spin frustrated systems

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Abstract. Rare-earth spin frustrated systems featured by strong spin-orbit coupling are distinctly different from their cousins built on 3d magnetic ions in many aspects. Rare-earth ions output a highly anisotropic magnetism which brings many exotic spin phases including quantum spin liquid, and can act as building blocks for a bond-dependent Kitaev spin system. In this talk, I will briefly introduce two rare-earth based spin frustrated families we revealed in recent years. One is the triangular lattice rare-earth chalcogenide $ARECh_2$ (A=alkali or monovalent ions, RE=rare earth, Ch=chalcogen) which appears as a large family of QSL candidates. The other one is van der Waals layered Kitaev spin system REChX (RE=rare earth, Ch=chalcogen, X=halogen). Our studies show that the two families offer an inspiring platform for exploring spin liquid phases, particularly Kitaev physics and its potential applications.

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CONTRIBUTED TALKS

Soft Cluster Crystals in Simulation and Experiment

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Abstract. Soft cluster crystals are unconventional state of matter, characterized with ordered periodic structures with multiple site occupancy. The number of overlapping building blocks in a cluster at each lattice site is not fixed but its expectation value depends on thermodynamic conditions, which makes this exotic phase to be a hybrid of solidity and fluidity. Soft cluster crystals were first discovered in a model of penetrable spheres [1] and their first experimental realization is achived two decades later [2]. Here we show that experimental system that undergoes a phase transition from a cluster fluid to a body-centered-cubic cluster crystal and we disscuss theoretical background of its self-assembly processes [3,4].

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Unmovable Nodal Points and Lines in Two-Dimensional Materials: Dispersions and Positions in the Reciprocal Space

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Abstract. We have found all quasiparticles in non-magnetic, two-dimensional materials in the presence of time-reversal symmetry [1]. Analysis of all eighty layer groups, both single- and double-, indicates that nineteen sorts exist, which are located near high-symmetry points and lines in the Brillouin zone. Our results are presented graphically in analogy with space groups elements in International Tables for Crystallography. Our findings can pave the way towards realization of new 2D materials with unprecedent physical properties.

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Charge To Spin Conversion In Graphene On 1T-TaS_2 Monolayer Triggered By Charge Density Wave Proximity Effects

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Abstract. Proximity induced effects in graphene within van der Waals heterostructures provide highly promising systems for charge to spin conversion with further applications in spintronics. Here we will discuss the electronic properties of graphene on 1T-TaS_2 monolayer transition metal dichalcogenide. 1T-TaS_2 undergoes temperature controlled transition from normal phase to charge density wave phase and ferromagnetic state. Different phases in 1T-TaS_2 alter the low energy bands of graphene. We found that the formation of the charge density wave significantly enhances the Rashba angle [1]. The importance of the Rashba angle, introduced by a mechanical layer twisting within the van der Waals heterostructures, allows to involve of collinear charge to spin conversion mechanism. In the discussed case the charge density wave represents a platform for controlling of the exotic spin patterns in graphene involved in charge to spin conversion without a twist.

The work has been supported by the Slovak Academy of Sciences project project FLAG ERA JTC 2021 2DSOTECH, IMPULZ IM-2021-42, projects APVV-SK-CZ-RD-21-0114, VEGA 1/0105/20., and European Union's Horizon 2020 Research and Innovation Programme under the Programme SASPRO 2 COFUND Marie Sklodowska-Curie grant agreement No. 945478.

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ANALYSIS OF TWO-DIMENSIONAL CRYSTALS VIA RAINBOW SCATTERING

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Abstract. We present the results of our theoretical study of 5 keV proton transmission through two-dimensional crystals. Proton trajectories were obtained by numerical solving Newton's equations of motion. Obtained trajectories are subsequently used to construct the proton angular yield. Singularities of a function that maps initial proton positions to the set of scattering angles form lines in the scattering angle plane along which the angular yield is significantly larger. These lines are named rainbow lines in analogy with optical rainbow scattering. It is shown that the rainbow pattern determines the shape of the angular distribution of transmitted protons. Change in the interaction potential, due to reorientation of the crystal relative to the direction of the incident beam or by varying model parameters, induces nontrivial transformation of the rainbow pattern. We have conducted a thorough study of these transfigurations, which led to the development of the morphological analysis of rainbow scattering. The developed analysis technique is based on the study of shape, not the exact particle count or position of the rainbow line, which makes it insensitive to noise. An established morphological method was used for studying graphene thermal motion. The Debye theory and Molecular Dynamics were used to calculate the covariance matrix of atomic thermal vibrations. It was shown that the outer part of the rainbow pattern can be modeled by ellipses, whose parameters are dependent on the structure of the covariance matrix. A numerical procedure was developed to extract the covariance matrix from the corresponding outer rainbow lines. Furthermore, it was shown that the outer rainbows' size could be used to characterize the atomic composition of two-dimensional crystals. We have investigated the influence of a crystal structure on the rainbow pattern by studying the transmission of protons through graphene containing different point defects. It was shown that each defect type produces a distinctive rainbow pattern, which then could be used to determine the unknown densities of the different defect types present in the same sample.

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Observation of Many-Body Scarring in a Bose-Hubbard Quantum Simulator

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Abstract. Quantum many-body scarring has recently opened a window into novel mechanisms for delaying the onset of thermalization by preparing the system in special initial states, such as the Z_2 state in a Rydberg atom system. Here we realize many-body scarring in a Bose-Hubbard quantum simulator from previously unknown initial conditions such as the unit-filling state [1]. Our measurements of entanglement entropy illustrate that scarring traps the many-body system in a low-entropy subspace. Further, we develop a quantum interference protocol to probe unequal-time correlations, and demonstrate the system's return to the vicinity of the initial state by measuring single-site fidelity. Our work makes the resource of scarring accessible to a broad class of ultracold-atom experiments.

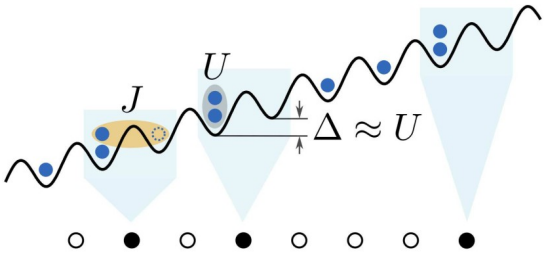

FIGURE 1. Mapping the PXP model onto a tilted Bose-Hubbard quantum simulator.

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A Nonequilibrium-Thermodynamics Perspective on Charge Separation in Organic Solar Cells

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Abstract. The operation of donor/acceptor (D/A) organic solar cells (OSCs) leans on the separation of the strongly bound charge transfer exciton (CTE) localized at the D/A interface into free charges [1]. Kinetic considerations suggest that CTE separation is facilitated by a combination of charge delocalization and moderate disorder [2], while it is hampered by strong disorder [2] and/or strong interaction with phonons [3]. From the standpoint of equilibrium thermodynamics, the charges in the CTE are thermodynamically free because its large binding energy is generally outweighed by the entropic contribution. While strong disorder and enhanced spatial connectivity eliminate the separation barrier [4], charge delocalization may increase it [5]. Such trends contradict the intuitive trends emerging from kinetic considerations.

We employ nonequilibrium thermodynamics to reconcile the kinetic and thermodynamic perspectives on charge separation in OSCs [6]. Within our one-dimensional model of a D/A interface [2, 3], we compute steady-state populations of interface states, which emerge from a competition between incoherent-light excitation, phonon-induced relaxation, and recombination. We then evaluate the nonequilibrium free-energy profile for charge separation and compare it to its equilibrium counterpart for different disorder strengths and delocalization extents. We find that the difference between the two profiles is maximized (minimized) when the separation efficiency is the largest (smallest). Our nonequilibrium profiles show that better delocalization suppresses the entropic contribution at small distances and enhances it at larger distances, meaning that charge delocalization promotes long-range separation. Despite the reduced dimensionality of our model, which is deleterious to the spatial connectivity of interface states, our nonequilibrium entropic contributions are consistently larger than the equilibrium ones because the former take into account the connectivity by phonon-assisted processes. Overall, we conclude that charge separation in the most efficient OSCs proceeds through a nonequilibrium pathway involving both the strongly bound CTE and higher-energy interface states.

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Spin Activity Correlations in Driven Disordered Systems

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Abstract. We study the spatio-temporal correlations in the spin flipping activities of the disordered systems realized within the frame of the field-driven three-dimensional zero-temperature nonequilibrium random field Ising model (ZT NEQ RFIM). Our results for the spatial activity correlations reveal that the rate-dependent scaling holds in the full range of rate regimes provided that the system parameters satisfy the finite-size and rate-dependent scaling conditions. Temporal activity correlations show high sensitivity to the driving, allowing the collapsing of waiting time distributions only in the limit of slow driving rates. These findings, based on extensive numerical simulations of large systems, reliably demonstrate the observed behavior and could be relevant for studies on various, particularly experimental, nonequilibrium systems driven at finite rates.

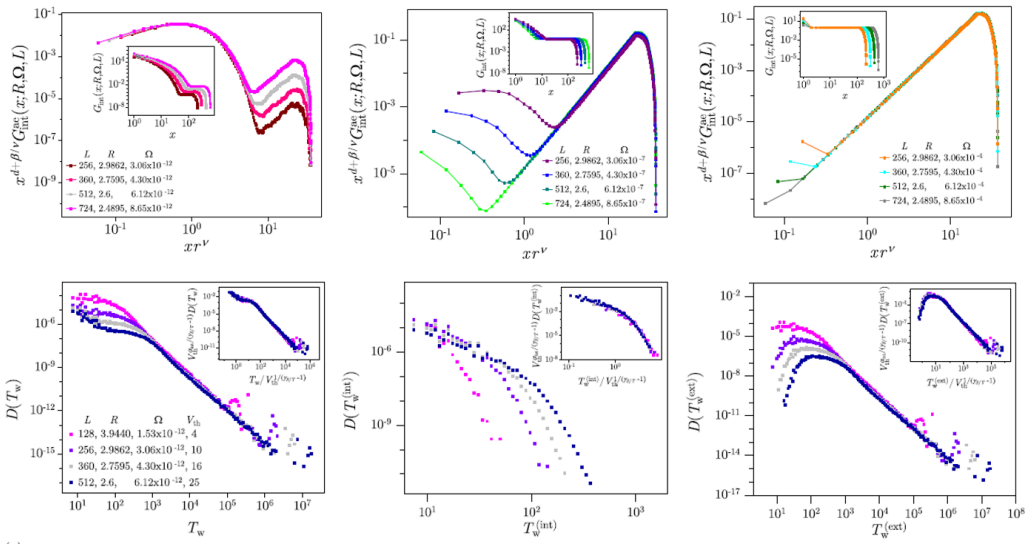

FIGURE 1. First row: Collapses of triggered activity correlation functions for systems whose parameters satisfy finite-size and rate-dependant scaling conditions. Second row: Distributions of waiting times (shown in main panels) accompanied with their collapses (given in pertaining insets) obtained for the case of slow driving regime.

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Higher-order Connectivity Patterns in the Correlation Structure of Complex Systems

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Abstract. Detecting pertinent patterns in the collective behavior of complex system elements is challenging for the practical, as well as theoretical, understanding of a system's dynamics. To date, complex network research set a convenient framework for modeling the complexity of systems formed by elements linked through pairwise interactions. However, this approach may neglect the effects of non-pairwise interactions [1], which produce higher-order structures that underlie complex systems [2], and higher-order interactions among large groups of elements are essential in the system's functioning and dynamics. On the other hand, one of the ways to capture pairwise weighted interactions of system elements is the formation of the cross-correlation matrix. Nevertheless, extracting grouped interactions of elements as higher-order correlations from pairwise is a rather challenging task [3] due to the nonlinearity of collective behavior which characterizes the system. Toward overcoming this problem, and as an approximation, we propose a framework for extracting collective behavior embedded in connectivity patterns based on pairwise interaction by aggregating elements into higher-order structures called simplices. These objects build non-trivial, complex, layered structures and display rich structural properties. In a nutshell, the development of a system reconstruction from correlations between its elements, using the algebraic topological approach, begins by mapping the system onto a multidimensional object called a simplicial complex [4]. We use the case of the financial system to exemplify the outcomes of the approach. Within this context, the k-order connected clusters of elements within the correlation structure represent aggregations of system elements (i.e., firms) under the criteria of induced multidimensional similarity, hence transcending the binary correlations. For example, 2nd order connected clusters of correlation structure represent groups of firms that form connected chains of elements where two successive firms are significantly correlated to three common firms. The interpretation of the results of these aggregations suits the qualitative classification of firms into groups due to the industry they belong. Furthermore, the novel and mixed collections of firms are revealed based on the algebraic topological approach applied. Our approach sheds light on the higher-order organization of interactions embedded in the cross-correlation matrix and, as a consequence, extracts patterns of collective behavior within a complex system.

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Proximity Induced Spin-Orbit Coupling In Phosphorene/WSe_2 and WSe_2/Phosphorene/WSe_2 van der Waals heterostructures

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Abstract. Two-dimensional materials and their der Waals heterostructures can be used to modify many properties of the target materials, via the proximity effect. Focusing on the heterostructure made of phosphorene and WSe_2 monolayer we reveal a strong transfer of spin-orbit coupling from WSe_2 monolayer to phosphorene. The common symmetry of the heterostructure is used to derive an effective spin Hamiltonian model for phosphorene and map to the data obtained using the first-principle calculations. We argue that the overall spin-orbit field is composed of the in-plane field, present when the horizontal mirror plane symmetry is broken, and the out-of-plane field, triggered by the broken out-of-plane rotational symmetry of the phosphorene monolayer. Finally, we show that the spin-orbit field can be controlled by twist of the layers and different encapsulation of phosphorene.

This project has received funding from the European Union's Horizon 2020 Research and Innovation Programme under the Programme SASPRO2 COFUND Marie Sklodowska-Curie grant agreement No. 945478, FLAG ERA JTC 2DSOTECH project, IMPULZ IM-2021-42, projects APVV-SK-CZ-RD-21-0114, VEGA 1/0105/20, National Center for Research and Development (NCBR) under the V4-Japan project BgapEng, APVV-21-0272, VEGA 2/0070/21, H2020 TREX GA No. 952165 project, Deutsche Forschungsgemeinschaft SFB 1277 (Project-ID 314695032, project B07), SPP 2244 (Project No. 443416183), and the European Union Horizon 2020 Research and Innovation Program under Contract No. 881603 (Graphene Flagship) and FLAG-ERA project 2DSOTECH.

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Evolution of Lattice, Spin, and Charge Properties Across $FeSe_{1-x}S_x$ Phase Diagram

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Abstract. It is widely believed that iron-based compounds host unconventional superconductivity. Among them in binary compound FeSe nematic and structural phase transition occurs simultaneously at 90 K and below 9 K superconductivity emerges. In isostructural and isoelectronic FeS, structural phase transition is not observed down to the lowest temperatures. By substituting selenium with sulfur atoms by approximately 20% a zero nematic phase transition temperature is reached suggesting the existence of quantum critical point (QCP). At this point T_c drops down to approximately 2 K [1]. By further increasing the sulfur content, the T_c increase up to 4 K for pure FeS. In order to investigate in which extent the properties and other instabilities of FeSe and FeS are interrelated, the entire substitution range of the $FeSe_{1-x}S_x$ was studied using inelastic light scattering technique. Data were taken as a function of sulfur concentration x for $0 \leq x \leq 1$, of temperature and of scattering symmetry. All types of excitations including phonons, spins, and charges are analyzed. It is observed that the energy and linewidth of the Fe-related B_{1g} phonon mode vary continuously across the entire range. The A_{1g} mode disappears above $x = 0.23$ and reappears at much higher energy for $x = 0.69$. In a similar way the spectral features appearing at finite doping in A_{1g} symmetry vary discontinuously. The magnetic excitation at approximately 500 cm^{-1} disappears above $x = 0.23$ where the A_{1g} lattice excitations exhibit a discontinuous change in energy. The low-energy mode associated with fluctuations displays maximal intensity at the nematostructural transition and thus tracks the phase boundary [2].

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Cumulant Expansion in the Holstein model: Spectral Functions and Mobility

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Abstract. The cumulant expansion (CE) method presents an alternative to the usual Dyson equation approach for the calculation of spectral functions and quasiparticle properties of interacting quantum many-particle systems. We examine the range of validity of this method by implementing it in a system described by the simplest electron-phonon model Hamiltonian - the Holstein model [1]. For a benchmark, we use the dynamical mean-field theory (DMFT) [2] which gives, as we have recently shown [3], rather accurate spectral functions in the whole parameter space. The results are also compared to the one-shot and the self-consistent Migdal approximation. While CE is exact in both the weak-coupling and the atomic limit, we find that even in a regime of intermediate coupling in 1D, the CE resolves well both the quasiparticle and the first satellite peak of the spectral function. CE also gives promising results for high temperatures, but it is not exact in the limit $T \to \infty$, which is proved analytically by analyzing the spectral sum rules.

Charge mobility μ is also calculated, using the bubble approximation of the Kubo formalism. At high temperatures, we demonstrate that it assumes a power law, which is different in the limit of weak coupling $\mu \propto T^{-2}$, and in the case of somewhat stronger coupling $\mu \propto T^{-3/2}$.

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Uniaxial Strain-Induced Changes in Vibrational Modes of FeSe

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Abstract. Strain application is an effective method for manipulating the characteristics of materials, and it proves particularly valuable in investigating the impact of local crystal structure changes on physical properties. Iron-based superconductors are ideal candidates for studying this strain dependence due to their heightened sensitivity to variations in crystal structure. Among these superconductors, FeSe stands out as a notable example that showcases the intricate relationship between superconductivity, magnetism, and electronic nematicity. This interplay can be adjusted through both chemical substitution and the application of physical pressure.
In this study, we present a comparison between first-principle calculations and Raman spectroscopy to examine the evolution of vibrational modes in strained FeSe superconductors. Using density functional theory, we conducted a comprehensive computational investigation on bulk FeSe crystals, subjecting them to in-plane uniaxial strain ranging from -2% to 2%. Our primary focus was to analyze the impact of straining the lattice constant and the resulting symmetry distortion on the distinctive A1g and B1g modes of FeSe. These numerical findings were then compared to experimental data obtained from Raman measurements, which allowed us to study the trends in changes of the A1g and B1g modes with applied strain.

Ion-atom interaction potential dependence on the ion's charge exchange

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Abstract. It was both shown theoretically and experimentally that it was possible to construct an accurate proton-silicon interaction potential (the rainbow potential) applying the rainbow morphological method[1]. That method has been also introduced for studying ion-atom interaction potentials for different ion-crystal combinations[2-4]. In the work presented here, we analyze the proton-silicon interaction potential dependence on the changing of the charge of neon atoms inside the silicon <100> crystal channels. It has been demonstrated that one can prescribe the rainbow potential dependence on the ion's charge state.

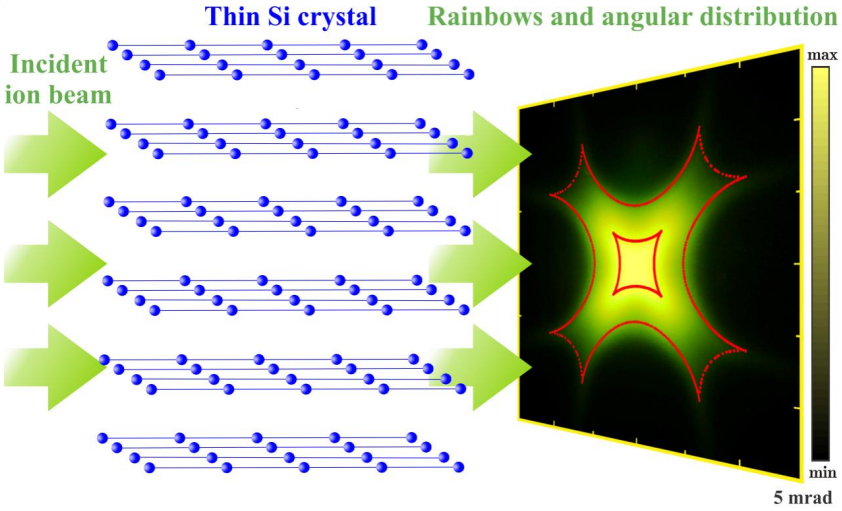

FIGURE 1. Transmitted ions angular distribution and the corresponding rainbow pattern

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The Anisotropic Interlayer Exchange In Van Der Waals 2D Magnets

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Abstract. Combining the density functional theory calculations with Hamiltonian modelling and symmetry analysis, we study the anisotropic interlayer exchange in bilayer CrI_3 [1]. To calculate the anisotropic interlayer exchange that is usually an order of magnitude smaller than the isotropic Heisenberg exchange, we develop an accurate computational procedure that can be applied to any two-dimensional (2D) magnetic heterostructure. We find a considerable interlayer Dzyaloshinskii-Moriya (DM) and an order of magnitude smaller Kitaev interaction between the layers' sublattices. Our finding demonstrates the ability of iodine ligands to efficiently mediate the interlayer DM interaction owing to their delocalized 5p orbitals that feature strong spin-orbit coupling. In addition, we show that the single-ion anisotropy, that is usually perceived as the magnetic property inherent of monolayer, largely depends on stacking and increases by 50% from monoclinic to rhombohedral bilayers. Our study gives promise that semiconducting magnetic van der Waals heterostructures can be employed for the chiral control of spin textures, similar to what is experimentally realized only with metallic ferromagnetic thin films [2].

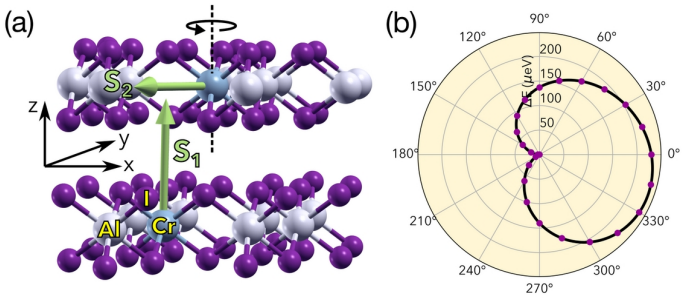

FIGURE 1. (a) Perpendicular spins of two nearest Cr neighbors from different layers in monoclinic bilayer CrI_3. Spin $\mathbf{S_1}$ is fixed along the z-axis while $\mathbf{S_1}$ is rotating around it. (b) The energies obtained from DFT calculations (purple points) are fitted to bilinear spin Hamiltonian (black cardioid curve).

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Solving the puzzle of magnetic 2D materials – from electronic structure to magnetic interactions

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Abstract. Since 2017 and the first experimental validations of long-range magnetic order in two-dimensional (2D) materials **[1,2]**, the fields of theoretical **[3-4]** and experimental **[5-6]** studying of magnetic 2D materials (M2DMs) have received much attention of the scientific community. For a long time – the thirteen years since the discovery of the first 2D material, graphene – nobody considered the possibility of long-range magnetic order existence in 2D, due to the Mermin-Wagner theorem. The constraint imposed by this theorem – that the long-range magnetic order cannot survive in 2D if system hosts only isotropic magnetic interactions – is circumvented by the strong anisotropic interactions present in M2DMs. However, despite the facts that there is large number of theoretical studies of M2DMs in past few years, and that physical mechanisms giving rise to magnetic interactions between atoms are known – direct exchange, superexchange, Goodenough-Kanamori-Anderson (GKA) rules – a little is known about how much particularly each of the physical mechanisms contributes to the magnetic order in 2D material of interest. Moreover, after thorough search through the literature, one may think that this question is being either neglected, or at best addressed in a descriptive manner, without concrete quantification, with some exceptions **[7]**. This gap in the literature has motivated me to study the physical origin of the magnetic interactions in 2D materials. As the first platform, I have chosen the virtual, square-lattice, M2DM consisting of equal amount of transition metal (TM) and nonmetal (L) atoms – ligands and isotropic interactions in it. I have discovered that superexchange dominates the process of magnetic exchange and that even orbital occupation of non-magnetic L atoms plays important role in the sign and size of magnetic interactions between TM atoms.

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Exploring Superconductivity In Doped Mono- And Bilayer Borophenes

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Abstract. The boron atom, possessing a profound research background, persists in engrossing the scientific community through its extraordinary and distinguishing chemical properties [1]. During the initial stage of boron exploration, the primary aim entailed comprehending the fundamental characteristics of this lightweight element through meticulous examination of its behavior in various dimensions, primarily encompassing three-dimensional (3D) clusters and the potential formation of two-dimensional (2D) structures [2,3]. Expanding upon previous theoretical predictions [4,5], a significant advancement was achieved in 2015, marked by the synthesis of two-dimensional (2D) boron configurations on a silver substrate, which were subsequently denoted as borophenes [6,7]. This pivotal advancement has enabled a plethora of research endeavors, elucidating the distinctive physical properties inherent in this anisotropic metallic material. These properties include high mechanical flexibility and strength, optical transparency, the existence of Dirac fermions, and the theoretically predicted superconductivity. The diverse array of physical properties exhibited by borophene make it exceptionally well-suited for a wide range of advanced technological applications, encompassing, but not limited to, energy storage, gas sensing, catalysis, and the fabrication of nano-superconducting devices [8, 9]. Nevertheless, the practical utilization of borophene has been hindered due to its susceptibility to oxidation upon contact with air, resulting in the loss of its potentially beneficial functional properties [10]. Significant progress has been achieved in addressing this issue through the synthesis of hydrogenated borophene (borophane) [11] and various polymorphs of bilayer borophene [12,13]. Hydrogenation effectively mitigates the undesired reactivity of borophene, while bilayer structures exhibit reduced susceptibility to oxidation compared to their monolayer counterparts. Drawing inspiration from recent advancements, I will present the advantageous impacts of hydrogenation on the superconducting properties of monolayer borophenes. Additionally, I will explain the role of intercalation in stabilizing and augmenting phonon-mediated superconductivity in bilayer borophenes. The primary objective is to comprehend the superconducting properties exhibited by these structures, which possess stability in ambient conditions (outside the vacuum chamber) and demonstrate minimal chemical reactivity. This renders them highly suitable for the development of advanced nano-superconducting devices.

$Mo_xW_{x-1}S_2$ Nanotubes For Advanced Field Emission Application

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Abstract. Individual multiwalled WS_2 and MoS_2 nanotubes (NTs) are having a resurgence of interest, as interesting optical and electrical properties have been reported in recent years [1, 2]. On the other hand, nanotubes have been vastly neglected as possible alloyed transition metal dichalcogenides (TMDC). Most of the research so far, both theoretically and experimentally, focused on flat, two-dimensional structures, with only a few reports that focused on non-carbon-based alloyed NTs [3]. Additionally, TMDCs have opened a new frontier in the area of field emission devices, due to their layered structure and the presence of thin and sharp edges with high aspect ratios which enhance the local electric field.In this work, we present highly crystalline multiwalled $Mo_{1-x}W_xS_2$ NTs grown with the chemical vapour transport method [4]. Energy-dispersive X-ray spectroscopy, Raman spectroscopy, and X-ray diffraction indicate that the molybdenum and tungsten atoms are randomly distributed within the crystal structure and that the material is highly crystalline. High resolution TEM and electron diffraction (ED) patterns further corroborate these findings. A detailed analysis of the ED patterns from an eight-layer nanotube revealed that they grow in the 2H structure, with each shell consisting of one bilayer. The work function of the NTs is comparable than that of pure MoS_2 and lower of pure WS_2 NTs, making them ideal candidates for field emission applications. Two devices with different geometrical setup were prepared and tested as field emitters, showing promising results for single nanotube field emission applications.

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Single-Molecule Probing By Rectification in a Nanogap

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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 single-molecule detection. Also, we suggest the application of nitrogen-terminated graphene or CNT nanogaps due to their inherent outstanding features. With 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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POSTER SESSION

Crystal structure and phase transitions in $InSiTe_3$

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Abstract. Although first report of $InSiTe_3$ single crystal synthesis and its structure dates nearly 30 years ago, only a few studies are available up till today. Unlike its related compounds ($CrSiTe_3$, $CrGeTe_3$) which have been intensively studied, and their high and low temperature physical properties are well established, only resistivity and thermal conductivity, as well as theoretical predictions of thermodynamical and mechanical stability of $InSiTe_3$ were investigated. Probably, one of the main issues causing lack of research data is the proper determination of $InSiTe_3$ crystal structure, since the literature predicts three different space groups for this material, $P3$, $P\bar{3}$, and $P\bar{3}1m$.

In order to properly investigate $InSiTe_3$ crystal structure we employed inelastic light scattering technique, and DFT calculations for all suggested crystal structures. Six out of eight and seven out of ten Raman active modes for proposed $P\bar{3}1m$ and $P\bar{3}$ space groups, respectively, are observed and assigned, in agreement with numerical calculations. The theoretical calculations for $P3$ crystal structure are in a strong discrepancy with theoretical results, hence this proposed space group can be neglected. The obtained results suggest the coexistence of two triagonal crystal phases, high symmetry one, $P\bar{3}1m$ and low symmetry $P\bar{3}$ space group. Additionally, to the modes that are theoretically predicted, at around 500 cm^{-1} the A_{1g}/A_g "splitting" mode is detected. The appearance of this peak might be a consequence of local symmetry breaking due to a small difference in lattice parameters of both crystal phases. The temperature dependence of energies and linewidths of the most prominent Raman active modes show a monotonous decrease in energy and increase in linewidth when the material is heated from 80 K. At around 200 K discontinuities in phonon properties can be observed. Above the same temperature, additional features in Raman spectra between 175 and 300 cm^{-1} only in parallel scattering configuration are present, and may be a consequence of two-phonon processes. The phonon temperature dependence and these additional excitations indicate the presence of some kind of phase transition above 200 K. Due to the lack of theoretical and experimental studies the origin and type of this transition remains an open question and requires further analysis.

Effect of disorder and electron-phonon interaction on 2*H*-$TaSe_{2-x}S_x$ lattice dynamics

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Abstract. Quasi-2D materials have gained a significant attention in the last few years because of their unique physical properties. The family of transition metal dichalcogenides is particularly intriguing due to their complex phase diagrams, characteristic optical properties and possibility to observe collective electron phenomena at higher temperatures. A strong correlation was observed between the electron-phonon interaction and the CDW phase in materials that display such states. Recent study has revealed that crystalline disorder promotes superconductivity while simultaneously suppresses CDW phase in metallic single crystal alloys of 2H-$TaSe_{2-x}S_x$.

Raman spectroscopy was used to investigate the effect of defects on lattice dynamics and electron-phonon coupling in these materials, and the results were compared to theoretical calculations. In our scattering configuration two out of four Raman active modes predicted by symmetry for parent compounds are identified. Additionally, in the spectra of pure samples broad two-phonon structures are observed, emerging as a consequence of strong electron-phonon coupling in related phonon branches. By substituting Se with S atoms, extra peak obeying A_{1g} selection rules, overtone in nature, appears in spectra along with an intriguing evolution of two-phonon structure. The Raman spectra of the $x = 0.84$ sample shows single-phonon excitations that are superimposed on already existing structure. These excitations correspond to PDOS maxima projected due to significant crystallographic disorder. Symmetry predicted A_{1g} modes expectedly harden with doping as unit cell volume decreases, whereas E_{2g} modes exhibit anomalous behavior attributed to enhanced electron-phonon coupling. The analysis of E_{2g} mode Fano parameter indicates that disorder has a minor impact on electron-phonon interaction.

Classification of complex networks with graph neural networks: importance of network properties and limitations

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Abstract. Graph neural networks (GNNs) have emerged as a powerful tool for machine learning on graph structures, offering great potential for solving a wide range of problems in complex network theory, physics, and chemistry. However, the interpretability of GNNs remains a challenge, as they often function as black boxes, making it difficult to understand the underlying decision-making process. In this work, we delve into the black box of GNNs to investigate their classification capabilities and how they depend on network structure and explore the interpretability of their results. We employ multiple GNN models to perform classification tasks between Erdős-Rényi (ER) and Barabási–Albert (BA) graphs to initiate our investigation [1]. We use different GNN architectures and hyperparameters to compare these models' performances and results. During the GNN training process, we utilize network properties as features and employ GNNExplainer to identify the most influential features driving the classification between these distinct graph structures.

Building upon these initial insights, we extend our study to explore the behavior of GNN models in classifying different dk-random graphs. Specifically, we train multiple GNN models with different architectures and hyperparameters to classify 0k, 1k, and 2k random graph structures for four existing real-world networks (the Internet, US airport network, human protein interactions, and techno-social web of trust) [2]. We leverage the knowledge of the differences between 0k, 1k, and 2k graphs, along with variations in network properties observed in these structures for different real-world networks, to interpret and analyze the results from GNNExplainer. Our findings underscore the significance of different network properties in distinguishing between graph structures (ER/AB and 0k/1k/2k) for different GNN models and networks. Furthermore, we gain insights into the limitations associated with this approach, facilitating a comprehensive understanding of the interplay between GNNs, network properties, and graph structure classification.

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TiO_2/PMMA nanocomposites functionalized with ascorbic and gallic acid for environmental applications

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Abstract. Enhancing water quality and purification can have a significant positive impact on human well-being and the health of ecosystems. Photodegradation of wastewater using sunlight is very desirable since it can make this process more profitable, especially for large-scale applications. Here we report the study of TiO_2/PMMA nanocomposite foils surface modified with ascorbic and gallic acid and their combination. We investigate the effect of surface modification on the photocatalytic efficiency of nanocomposite foils under Simulated Solar Irradiation. Surface modification of nanocomposite foils leads to the formation of a colored surface complex in the color range from light orange to brownish orange. This leads to red shift of the absorption threshold of TiO_2, which enhances the utilization of solar irradiation. Scanning electron microscopy (SEM), UV/Vis spectroscopy, Fourier transform infrared (FTIR) spectroscopy and photodegradation experiments were performed to evaluate the effect of surface modification of nanocomposites. This green and straightforward technique for producing surface-modified TiO_2/PMMA nanocomposite foils can be employed to create versatile photocatalysts suitable for energy conservation and environmental preservation in a wide range of applications.

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Lattice dynamics and phase transitions in $Mn_3Si_2Te_6$

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Abstract. Quasi-two-dimensional materials, known for their easy exfoliation to a monolayer and unique optical and transport properties, create a platform for experimental investigation of various low-dimensional phenomena, such as low-dimensional magnetism. This, together with their potential application in spintronics, nanoelectronics, data storage, biomedicine, and as a platform for magneto-optoelectronic devices puts these materials in the center of extensive experimental studies. Aiming to provide much needed deeper insight into these systems, we have investigated the vibrational properties of ferrimagnetic $Mn_3Si_2Te_6$ single crystals using Raman spectroscopy. Fourteen out of eighteen Raman-active modes were observed in our spectra and assigned according to the trigonal symmetry. Additional peaks, which obey the A_{1g} selection rules, were attributed to the overtones. The obtained experimental results were compared to the density functional theory calculations and found to be in a good agreement. The temperature evolution of phonon properties of the two most prominent peaks reveal three subsequent, possible magnetic, phase transitions at T_1= 142.5 K, T_2= 190 K, and T_3= 285 K which have significant impact on the strength of the spin-phonon interaction in $Mn_3Si_2Te_6$. These are likely caused by the competition between the various magnetic states, close in energy. This research provides comprehensive insight into the lattice dynamics, and gives arguments to support the existence of competing short-range magnetic phases in $Mn_3Si_2Te_6$.

Quantum Entanglement and Quantum Coherence Correlations in XY Spin Chains

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Abstract. Quantum entanglement and coherence have attracted significant attention recently. These properties arise from quantum superposition, prompting the exploration of potential correlations between them. This poster examines the correlation in different systems with varying anisotropy, specifically XY spin chains with the Dzyaloshinskii-Moriya interaction. The quantum renormalization group method is employed to investigate the nature of this correlation and appearance of quantum phase transitions.

Acknowledgments. The authors acknowledge financial support of the Ministry of Education, Science and Technological Development of the Republic of Serbia (Grant No. 451-03-47/2023-01/200125).

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Dynamic-Polarization Forces Acting On A Charged Particle Moving Over A Graphene-Sapphire-Graphene Heterostructure

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Abstract. We investigate the stopping and image forces acting on an external charged particle moving parallel to a sandwich-like structure consisting of two graphene sheets separated by a layer of Al_2O_3 (sapphire), as depicted in FIG. 1. The effective dielectric function of the system is obtained using two descriptions of the electronic response of doped graphene: an *ab initio* method based on the time-dependent density functional theory calculations and an analytical expression based on the massless Dirac fermion (MDF) approximation for graphene π bands. It is found that the main discrepancies between the two methods come from the high-energy interband electron transitions, which are included in the *ab initio* method but not in the MDF method. Special attention is paid to the regime of low-particle speeds, where the MDF method compares well with the *ab initio* method, but the modeling is sensitive to the effects of finite temperature and the treatment of phenomenological damping. We also provide a semi-analytical analysis based on a modal decomposition of the energy loss function, for which we discuss the limit of a thick graphene-Al_2O_3-graphene structure.

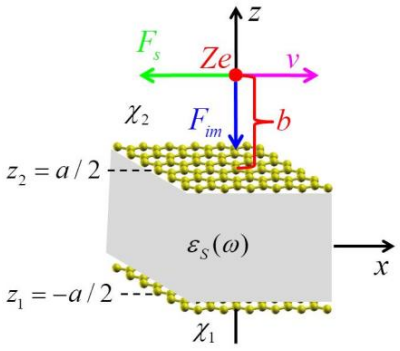

FIGURE 1. Diagram of the stopping force F_s and the image force F_{im} that act on the point charge Ze moving parallel to the x axis with constant speed v at a fixed distance b above the graphene-sapphire-graphene heterostructure. The polarization function of the top graphene layer placed in the $z_2 = a/2$ plane is χ_2 and of the bottom in the $z_1 = -a/2$ plane is χ_1. The Al_2O_3 layer of thickness a is described by local dielectric function $\varepsilon_s(\omega)$.

Magnetic Field Directed Assembly of Magnetic Non-Spherical Microparticles

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Abstract. Magnetic fields can generate orientation-dependent, long-range interactions between microparticles that direct their assembly into highly ordered structures. While much effort has been devoted to exploring the assembly of spherical microparticles[1,2], few reports have investigated the directed assembly of non-spherical magnetic microparticles[3,4]. Here, we use photolithography and soft lithography to fabricate anisotropically-shaped microparticles and follow their assembly in water suspension under the influence of a switching magnetic rotating field, i.e., a field that rotates 360° back and forth to suppress the net rotation of the particles. We investigate the assembly of up to five star-shaped microparticles with three and four arms. By using a simple numerical model, we interpret the results of the assembly process. Assembly of magnetic microparticles opens up exciting opportunities to engineer a variety of intriguing and complex architectures which are important in both fundamental science and technological applications.

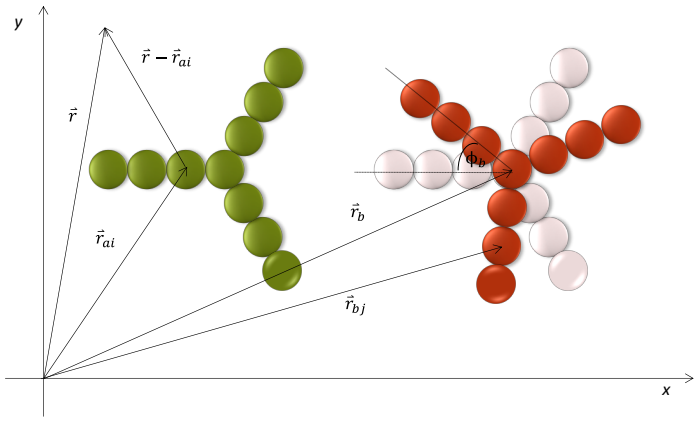

FIGURE 1. The numerical model describes each three-armed particle with ten-point dipoles: one in the center and three on each arm. The green particles represent the primary particle, while the red particles represent the test particle.

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Spin-wave Dispersion of a Layer Film With a Honeycomb Lattice

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Abstract. We consider a Heisenberg model of a layer film with a honeycomb lattice that has additional intralayer antiferromagnetic and interlayer ferromagnetic interactions. Dispersion relations for the acoustic and the optic branch are derived in the linear spin wave approximation and the negative energy solutions, which appear in the GF method, are interpreted by comparing the Klein-Gordon equation with the equations of motion of spin ladder operators.

A Method For Obtaining Holstein Polaron Mobility Using Real And Imaginary Time Path Integral Quantum Monte Carlo

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Abstract. Electron-phonon (e-ph) interaction is responsible for majority of transport phenomena in condensed matter. In this work, we consider the short-range (localized) e-ph interaction described by the Holstein Hamiltonian. We develop numerically exact path integral Monte Carlo (PIMC) method to obtain current-current correlation functions (CFs) and polaron mobility of one-dimensional Holstein model.

Generally, several challenges need to be overcome to reliably calculate dynamical properties using the PIMC methods. First one is the dynamical sign-problem of real time CFs which limits the real time QMC calculations to short real times. We were able to reduce the sign-problem to extent by appropriate choice of basis for representation of path integral which enabled us to calculate the real time CFs for longer times. On the other hand, the sign-problem can be completely eliminated by doing calculations in imaginary time and then analytically continuing to real time. The other challenge is that there is not a reliable method for analytic continuation of such numerically obtained values. We overcome these limitations by performing analytic continuation from imaginary and real time data combined which provides us with more reliable results compared to analytic continuation from purely imaginary time data.

For weak e-ph interaction strengths and temperatures that are not too low we were able to obtain real time CFs for long enough times by using PIMC algorithm derived from momentum representation of electronic degrees of freedom and coordinate representation of phonons. From such obtained CFs we were able to calculate polaron mobility with great accuracy by direct integration according to Kubo formula. For stronger interactions such an algorithm leads to a significant sign-problem for longer times and better results are obtained by using a different algorithm. In that case results are obtained by using PIMC algorithm derived from position representation of electronic degrees of freedom and coordinate representation of phonons to calculate real and imaginary time CFs. The polaron mobility is then obtained by analytic continuation from real and imaginary time data by singular value decomposition method. The method described enabled us to obtain polaron mobility for a range of temperatures and e-ph interaction strengths with a very small error.

Fe-nanoparticle-modified Langmuir-Blodgett Graphene Films for Pb(II) Water Purification

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Abstract. The surface of nonmagnetic Langmuir-Blodgett self-assembled (LBSA) graphene films is modified through structure engineering by chemical functionalization with Fe nanoparticles in order to induce local magnetic domains and investigate the application of such films for heavy metal water purification. We prepared and modified our films by single-step Langmuir-Blodgett procedure [1]. The influence of Fe-based magnetic nanoparticles on the structure and magnetic properties of LBSA films was examined by Raman spectroscopy, X-ray photoelectron spectroscopy (XPS), and Magnetic Force Microscopy (MFM). Raman and XPS confirmed the surface modification of the graphene films. Compared to an unmodified graphene film, which has no detectable magnetic response, MFM phase images show a strong phase shift difference compared to the substrate (~0.2°), indicating the presence of a local magnetic moment. In addition, we examined the use of magnetized LBSA graphene films for the adsorption of Pb(II) ions by immersing the films into Pb(II) solution. Results from XPS measurements depict the ability of modified films to detect and adsorb Pb(II) ions from water-based solutions. The development of a new generation of magnetic self-assembled 2D material films for heavy metal sensing and water purification that can overcome the deficiencies such as low purification efficiency, short-term stability, and high cost is of great interest for various applications in green technology.

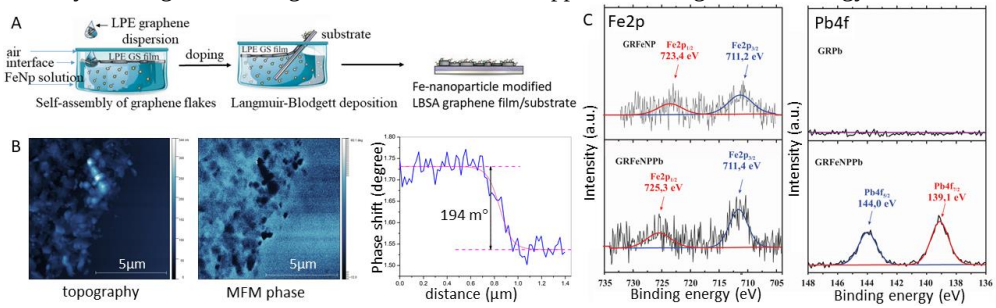

FIGURE 1. A) Fabrication of Fe-modified LBSA graphene films, B) AFM topography, MFM phase image, and representative MFM phase shift profile of Fe-modified LBSA films, C) XPS Fe2p spectra of modified films before and after interaction with Pb(II) ions, and Pb4f spectra of unmodified and modified films after interaction with Pb(II) ions.

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Effect of Laser Heating on Partial Decomposition of $Bi_{12}SiO_{20}$ (BSO) Single Crystals

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Abstract. In this study we present effects of laser heating on partial decomposition of BSO single crystals. The degree of decomposition directly depends on the power density and duration of the laser treatment, which is registered by the phonon spectra. After laser treatment, AFM measurements registered additional small spherical islands on the surface. Analysis performed on irradiated and non – irradiated samples showed significant changes in transmission spectra, XRD pattern, Verdet constant, magneto – optical properties and absorption coefficients. The material obtained after laser irradiation can be described as specific nanocomposites, consisting of bismuth – oxide and silicone – oxide – based nano – objects, which are arranged in a $Bi_{12}SiO_{20}$ matrix.

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Edge Solitons in Spiraling Waveguides

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Abstract. Spiraling propagation systems provide more interesting dynamics than their straight counterparts, because the centripetal force modifies the effect of potentials present and the interaction with the medium or other beams. Nonlinear light propagation in a spiraling waveguide array couples Bloch modes both within and between bands, and these non-inertial effects can lead to mode conversion, enhanced transport, and vector (gap) soliton formation [1]. Truncated rotating square waveguide arrays support localized (corner and central) modes that can exist even in the linear case [2]. On the other hand, edge states in a hexagonal array of helical waveguides are responsible for photonic 'topological insulation', in which light that propagates along the edges of photonic structures is topologically protected from scattering [3]. We intend to carry out detailed analysis of possible solitonic edge solutions in different spiraling waveguide arrays, by using Petviashvili's iteration method [4]. We will investigate the stability of these solutions by propagating them in the presence of defects.

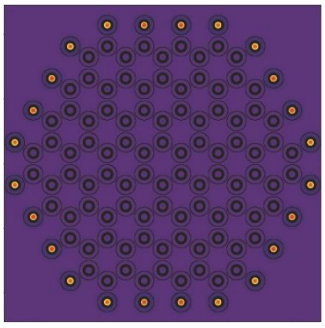

FIGURE 1. Edge soliton in a honeycomb photonic lattice.

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Cobalt Ferrite on Silicon Memristors: Device Fabrication and Resistive Switching Investigation

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Abstract. Memory resistors, or memristors, have a wide range of applications in numerous fields especially in the fields of resistive memory, cryptography, and neuromorphic computing. However multiple issues and challenges face the use of memristors in day-to-day operations. One such issue is the fabrication of these components using common, scalable practices. Here we present the sol-gel fabrication method, characterization procedure, and the results of the electrical characterization of a cobalt ferrite memristor fabricated on P++ silicon. A 100 nm cobalt ferrite layer facilitates the resistive switching in the memristor [1]. The silver layer acts as a top electrode, while the silicon base acts as a bottom electrode. These electrodes are active and help to replenish the resistive switching process with adding positive charges. These charges, along with oxygen vacancies caused by defects in the cobalt ferrite layer, form conductive channels that get damaged through Joule heating, enabling the resistive switching mechanism of the memristor [2]. The analysis of the current-voltage *I-V* loops shows different conduction mechanisms during the low resistive state the high resistive state [3].

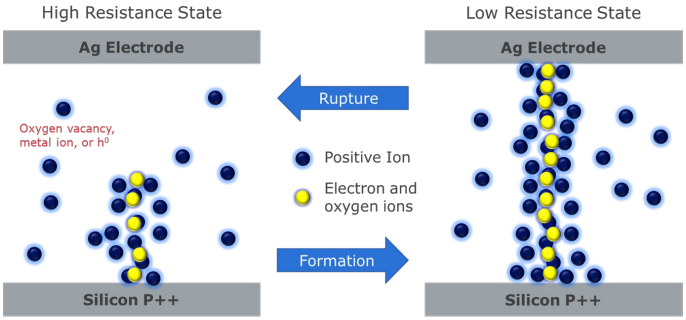

FIGURE 1. Resistive switching is facilitated by the formation and destruction of conducting filaments formed in the cobalt ferrite layer.

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Impact of Interface Diffusion and Doping Segregation on Transport Characteristics in THz Quantum Cascade Lasers

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Abstract. Quantum cascade lasers (QCLs) are unipolar semiconductor lasers with flexible emission wavelengths that can be engineered by variation of semiconductor layer thicknesses and composition. QCLs were first demonstrated in 1994. [1] and are typically created by molecular beam epitaxy. Due to the high temperature of the molecular beam at which this growth occurs, the created interfaces between different materials are not abrupt, which is a common approximation, but are rather subject to the diffusion of the barrier material, which changes the material composition of the interfaces. It was recently shown that this compositional (interface) diffusion can have a prominent effect on the maximum operating temperature of a THz QCL [2]. Doping segregation, that is the diffusion of the charged dopants, is an effect that is also present in real QCLs and can be of interest when modelling QCLs as it changes the Hartree term in the total effective potential energy, and in turn the electronic structure. In this work we investigate the impact of interface diffusion and doping segregation on transport characteristics, such as material gain and current density in THz QCLs, while varying the externally applied electric field along the growth direction. For calculating the transport characteristics, we used the density matrix model presented in [3]. Diffusion was modelled by numerically solving Fick's law with the finite distance method, and the results were in agreement with the analytical error function results presented in [4].

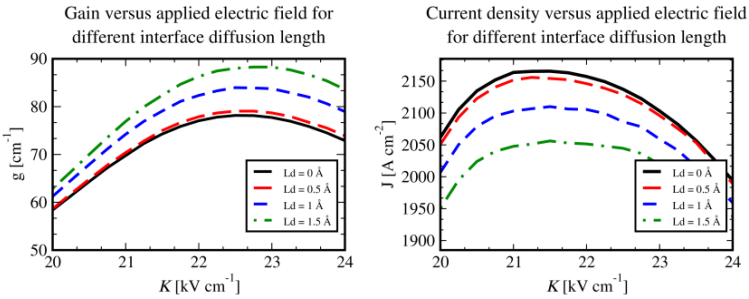

FIGURE 1. Effect of interface diffusion on material gain and current density in quantum cascade laser

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ACKNOWLEDGMENT

This work was financially supported by the Ministry of Science, Technological Development and Innovation of the Republic of Serbia under contract number: 451-03-47/2023-01/200103, "Multi-Scale Modeling of Terahertz Quantum Cascade Laser Active Regions", Multilateral scientific and technological cooperation in the Danube region 2020-2021, "DEMETRA: Development of high-performance mid-IR / THz quantum cascade lasers for advanced applications", Science Fund of the Republic of Serbia, Serbian Science and Diaspora Collaboration Programme: Knowledge Exchange Vouchers, and European Cooperation in Science and Technology (COST) Action CA21159 PhoBioS.

Localized Waves in Graphene Metamaterials

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Abstract. Dynamics of the propagation of terahertz relativistic spatial solitary waves in doped graphene metamaterials is governed by the nonlinear equation [1]: $i\,\partial\psi/\partial z + \Delta\psi - \psi/(1+|\psi|^2)^{1/2} = 0$, where ψ is the wave function and Δ is the transverse Laplacian operator. The same square-root saturable intensity dependence describes accurately the most relevant contribution of the space-charge field in two transverse dimensions in the photorefractive crystals [2, 3, 4]. The solitary solutions can be found from the previous equation by using the modified Petviashvili iteration method [5, 6] for finding eigenfunctions and eigenvalues of elliptic boundary-value problems. The fundamental soliton solution is of the form $\psi(x,y,z) = u(x,y)\,e^{i\mu z}$, where μ is the propagation constant (or an eigenvalue) and the real-valued amplitude function $u(x,y)$ satisfies the following elliptic partial differential equation: $-\mu u + \Delta u - u/(1+|u|^2)^{1/2} = 0$. Possible axially symmetric solitonic solutions, characterized by n zeros at finite radial distance r, are presented in Fig. 1 (left). The fundamental soliton (n=0) is the stable solution: perturbed ground-state soliton approaches its stationary state very quickly, Fig. 1 (right). But, in real physical systems things are not so simple. We intend to improve this model by including dissipative terms in the propagation equation, as well as by introducing other interaction mechanisms.

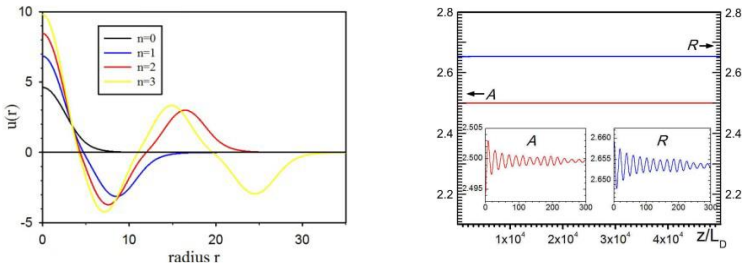

FIGURE 1. Profiles of axially symmetric solitonic solutions (characterized by n zeros at radial distance r) for μ=-0.5 (left). Propagation of perturbed fundamental soliton (n=0) for μ=-0.7: amplitude A and beam radius R oscillate only in the beginning (right).

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Long-term effects of abrupt environmental perturbations in model of group chase and escape with the presence of non-conservative processes

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Abstract. This paper examines the influences of environmental perturbations on dynamical regimes of model ecosystems. We study a stochastic lattice model describing the dynamics of a group chasing and escaping between predators and preys. The model include smart pursuit (predator to preys) and evasion (preys from predators). Both species can affect their movement by visual perception within their finite sighting range. Non-conservative processes that change the number of individuals within the population, such as breeding and physiological dying, are implemented in the model. The model contains five parameters that control the breeding and physiological dying of predators and preys the birth and two death rates of predators and two parameters characterizing the birth and death of preys. We study the response of our model of group chase and escape to sudden perturbations in values of parameters that characterize the non-conservative processes. Temporal dependencies of the number of predators and preys are compared for various perturbation events with different abrupt changes of probabilities affecting the non-conservative processes.

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Strain-Controlled Electronic and Optical Properties of hBN/InTe and hBN/GaTe Heterostructures

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Abstract. Van der Waals heterostructures have been extensively researched recently, as their rich physics and new effects not present in their component materials alone, make them prominent for applications in modern nanodevices [1,2]. The application of strain provides more flexibility to tune the properties of such structures, as well as to utilize them in devices such as precise sensors and detectors [3]. Here we present the study of novel hBN/InTe and hBN/GaTe heterostructures under biaxial strain, which are previously shown as an excellent broad-spectrum absorbers [4]. Using density functional theory, we investigate the effect of strain on their electrical and optical properties. We demonstrate how the strain can influence the electronic structure and allow the fine-tuning of the band gap. The absorption spectrum changes accordingly, enhancing specific parts of the absorption function with different strain intensities.

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Tunnel Junction Sensing of TATP Explosive at the Single-Molecule Level

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Abstract. Triacetone triperoxide (TATP) is a homemade, potent explosive and, unfortunately, is used in many terrorist attacks. It is hard to detect, and present techniques for its sensing do not offer portability. Fortunately, TATP is volatile, and gas-sensing-based devices for TATP detection would provide a higher level of safety. Here, we explore the possibility of single-molecule TATP detection in the air by tunneling current measurement in the N-terminated carbon-based nanogaps, at the DFT+NEGF level of theory. We found TATP averaged current amplitude of tens nano amperes, with a discrimination ratio with respect to prevalent indoor volatile organic compounds (VOC) of a few orders of magnitude. That high tunneling current is due to specific TATP HOMO contributions to electronic transport. The transport facilitates the strong, in-gap electrical field generated by N-C polar bonds from electrode ends and TATP-electrode hybridization, spurred by oxygen atoms from a probed molecule.

Conductivity of Cold Bosonic Atoms in Optical Lattices

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Abstract. Cold atoms in optical lattices provide a clean realization of the Hubbard model. While the focus of early experiments was on understanding quantum phase transitions driven by the interplay of hopping and local interactions [1], more recent experiments aim at studying quantum transport in these setups. The onset of bad-metal behavior, characterized by the resistivity linear in temperature, has been investigated recently [2, 3]. While the conductivity of of the fermionic version of the model has been addressed in much detail both from the theoretical and experimental perspective, far less is known about transport in the bosonic version [4]. We investigate conductivity in the strongly-interacting regime of the Bose-Hubbard model. We address the high-temperature regime and use numerically exact calculations for small lattice sizes. At weak tunneling, we find multiple peaks in the optical conductivity that stem from the Hubbard bands present in the many-body spectrum. This feature is slowly reduced as the tunneling rate gets stronger. Further, we find the regime of linear resistivity. When the interactions are very strong, the leading inverse-temperature coefficient in conductivity is proportional to the tunneling amplitude. As the tunneling becomes stronger, this dependence takes quadratic form.

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