BOOK OF ABSTRACTS

ADVANCES
IN SOLID STATE PHYSICS
AND NEW MATERIALS
WORKSHOP
Spring 2026

ADVANCES IN SOLID STATE PHYSICS AND NEW MATERIALS

SPRING WORKSHOP 2026

May 25 - 29, 2026

Institute of Physics Belgrade

Belgrade, Serbia

CSSPNM
CENTER FOR SOLID STATE PHYSICS AND NEW MATERIALS

HIP-2D-QM

Funded by the European Union

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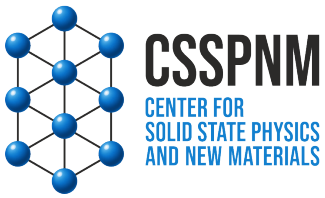


Advances in Solid State Physics and New Materials
Spring Workshop 2026

The international workshop ***Advances in Solid State Physics and New Materials – Spring Workshop 2026*** will take place from **May 25–29, 2026**, at the **Institute of Physics Belgrade (IPB)**, Serbia. The workshop is organized by the Center for Solid State Physics and New Materials, Institute of Physics Belgrade, as a continuation of the successful *Advances in Solid State Physics and New Materials* conference series.

The workshop aims to bring together researchers working in various areas of condensed matter and materials physics, with a particular focus on emerging quantum materials, low-dimensional systems, and advanced experimental and theoretical approaches in solid-state physics. The event will provide an opportunity for discussions, exchange of ideas, and strengthening of existing and future collaborations among researchers, postdoctoral fellows, and students.

Special emphasis of the workshop is placed on recent developments in:

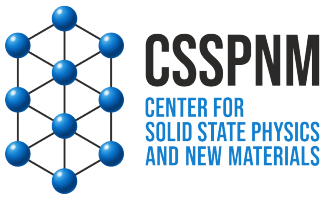
- Novel Quantum Materials
- Strong Correlations
- Ordering Phenomena and Phase Transitions
- 2D Materials and Interfaces
- Topology
- Magnetism
- Unconventional Superconductivity
- Soft Matter
- Semiconductors
- Polaron Physics
- And Other Relevant Topics

The workshop is organized within the activities of several ongoing international and national research projects conducted at the Center for Solid State Physics and New Materials, including the Horizon Europe ERA Chair project HIP-2D-QM (*Hidden Phases in 2D Quantum Materials*).

The scientific program will include invited lectures, contributed talks, and informal scientific discussions designed to encourage interaction between senior scientists and early-career researchers.

Workshop venue:
Institute of Physics Belgrade
Pregrevica 118, 11080 Belgrade, Serbia

Workshop website:
Advances in Solid State Physics and New Materials – Spring Workshop 2026



Advances in Solid State Physics and New Materials - Spring Workshop 2026 is organized by Center for Solid State Physics and New Materials at the Institute of Physics Belgrade (http://solidstate.ipb.ac.rs/), with support of European Union's Horizon Europe research and innovation programme (https://research-and-innovation.ec.europa.eu/) under grant agreement No. 101185375.

ADVANCES IN SOLID STATE PHYSICS AND NEW MATERIALS – SPRING WORKSHOP 2026

May 25 - 29, 2026, Institute of Physics Belgrade, Serbia

CONFERENCE PROGRAM

MONDAY, MAY 25

Time	Speaker	Title
9:00–9:30		**REGISTRATION**
9:30–9:50		**Opening remarks**
CHAIR	**Emil Božin**	
9:50–10:30	Vladimir Dobrosavljević	Mechanism of charge transfer and electrostatic field fluctuations in high-entropy metallic alloys
10:30–11:10	Vladan Stevanović	Effective bands and band-like electron transport in amorphous solids
11:10–11:30		**Coffee break**
CHAIR	**Vladimir Dobrosavljević**	
11:30–12:10	Rudi Hackl	Light Scattering in Novel Quantum Materials
12:10–12:30	Jovan Blagojević	Disorder and Electron–Phonon Coupling in 2H-$TaSe_{2-x}S_x$ Probed by Raman Spectroscopy
12:30–12:50	Tea Belojica	Experimental Evidence of Coherent-Like Phonon State in $InSiTe_3$
12:50–13:30	Nenad Lazarević	Phonon Response of FeSe Under Uniaxial Strain
13:30–14:30		**Lunch break**
CHAIR	**Rudi Hackl**	
14:30–15:10	Alexey Minenkov	Unraveling Material Evolution at the Nanoscale via in situ and ex situ Transmission Electron Microscopy
15:10–15:50	Bratislav Lukić	Neutron Imaging at ILL: Expanding Capabilities for Operando and Multi-Scale Materials Characterisation
15:50–16:30	Nataša Lazić	Spin Crystallographic Groups and Magnetic Arrangements in Low-Dimensional Structures
16:30–17:10	Božidar Nikolić	Electron-phonon Decoupling in Kagome Lattice

40-minute talks: 30 min presentation + 10 min Q&A / 20-minute talks: 15min presentation + 5 min Q&A

TUESDAY, MAY 26

Time	Speaker	Title
CHAIR	**Jernej Mravlje**	
9:30–10:10	Cesare Franchini	Hidden orders and polaron effects in spin-orbit entangled correlated insulators
10:10–10:50	Michele Reticcioli	Dual Role of Polarons in Functional Materials
10:50–11:10		**Coffee break**
CHAIR	**Cesare Franchini**	
11:10–11:50	George Volonakis	Ab initio Modelling and Computational Screening of Halide Perovskites to Ternary Halide Double Salts
11:50–12:30	Jernej Mravlje	Breakdown of Drude transport and origin of c-axis resistivity maximum in layered oxides
12:30–12:50	Lorenzo Ciliberti	Machine Learning the Order-Disorder Jahn-Teller Transition in $LaMnO_3$
12:50–13:30	Mario Novak	Colossal magnetoresistance in insulating $EuCd_2As_2$
13:30–14:30		**Lunch break**
CHAIR	**Mario Novak**	
14:30–15:10	Emil Božin	Hidden States and Dimensionality Reduction as Enablers of Ultralow Thermal Conductivity
15:10–15:50	Ana Milosavljević	Strain-Tunable Hysteresis of the CDW Transition in Bulk 1T-TaS_2
15:50–16:10	Ana Kanjevac	Evolution of Electron-Phonon Coupling Across a Topological Phase Transition in $ZrTe_5$

WEDNESDAY, MAY 27

Time	Speaker	Title
CHAIR	**Željko Šljivančanin**	
9:30–10:10	Masahiko Isobe	Exotic Phase Transitions in Chromates with Mixed Valence
10:10–10:50	Carl Lehman	Probing Green's Function Zeros by Co-tunneling through Mott Insulators
10:50–11:10		**Coffee break**

40-minute talks: 30 min presentation + 10 min Q&A / 20-minute talks: 15min presentation + 5 min Q&A

CHAIR	**Andrey Mishchenko**	
11:10–11:50	Oleg Yazyev	In Silico Discovery of Novel Topological Materials
11:50–12:10	Lenka Filipović	Electronic Properties of Layered Phyllosilicates: A First-Principle Analysis
12:10–12:50	Željko Šljivančanin	Stabilization of Single Atoms on 2D Materials: From Hydrogen Catalysis to Atomic-Scale Magnetism
12:50–13:50		**Lunch break**
CHAIR	**Carl Lehman**	
13:50–14:30	Petar Mitrić	Transport in electron-phonon systems: insights from the model systems
14:30–15:10	Stefano Ragni	Polarons with Nonlinear Electron-Phonon Coupling via Diagrammatic Monte Carlo in Displacement Space
15:10–15:50	Andrey Mishchenko	Diagrammatic Monte Carlo: exact solution of electron-phonon and Kondo-Lattice problem
15:50–16:10	Samuele De Amicis	Diagrammatic Monte Carlo for Anisotropic and Degenerate Bands

THURSDAY, MAY 28

Time	Speaker	Title
CHAIR	**Dejan Đokić**	
9:30–10:10	Armando Consiglio	Room-Temperature Excitons and Exciton Dispersion in a Two-Dimensional Quantum Spin Hall Insulator
10:10–10:50	Sonja Predin	Zitterbewegung Chirality and Its Relation to Berry Curvature
10:50–11:10		**Coffee break**
CHAIR	**Armando Consiglio**	
11:10–11:50	Milorad Milošević	
11:50–12:30	Dejan Djokić	Fano Universality Revisited: Phonon Decoupling as a Pathway to Expedient Raman Spectral Analysis
12:30–13:10	Milena Filipović	Transport Through a Junction With a Precessing Anisotropic Molecular Spin
13:10–13:50	Zorica Popović	Andreev bound state spectrum and nonreciprocal Josephson current in SFFS junctions with interfacial SOC
13:50–14:50		**Lunch break**

40-minute talks: 30 min presentation + 10 min Q&A / 20-minute talks: 15min presentation + 5 min Q&A

CHAIR	**Jelena Pešić**	
14:50–15:30	Biljana Kosanović	Open Science in Serbia: Not a Fairy Tale, but a Good Case Study
15:30–16:10	Matija Zlatar	The Serbian Reproducibility Network: Building Reliable and Open Research Practices in Serbia
16:10–16:30		**Open Science Panel Discussion**

FRIDAY, MAY 29

Time	Speaker	Title
CHAIR	**Jelena Mitrić Otašević**	
9:30–10:10	Snežana Lazić Knežević	Cost-Efficient Deterministic Engineering of Quantum Light Emitters in Two-Dimensional Semiconductors
10:10–10:50	Sanja Đurđić Mijin	Why are photonic qubits based on deterministic quantum light sources key to future quantum technologies and how can we engineer them for practical applications
10:50–11:10		**Coffee break**
CHAIR	**Sanja Đurđić Mijin**	
11:10–11:30	Borislav Petrović	Interband Cascade Lasers With Hybrid Superlattice Plasmon-Enhanced Claddings For Operation Beyond the Sweet Spot Wavelength Range
11:30–11:50	Jovana Jelić	Spectroscopic and Structural Characterization of Co(III), Cu(II), and Ni(II) Complexes with the Bioactive Hp_2DAP Ligand
11:50–12:30	Jelena Mitrić Otašević	Processing-Dependent Aging Behavior of Dental Resins: How Surface and Molecular Structure Dictate Color Stability and Translucency
12:30–13:30		**Lunch break**

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Hidden States and Dimensionality Reduction as Enablers of Ultralow Thermal Conductivity

Emil S. Bozin[a]

[a]*Center for Solid State Physics and New Materials, Institute of Physics Belgrade, Serbia*

Abstract. Nanoscale symmetry breaking and dynamic structural fluctuations critically govern the behavior of complex quantum materials, yet often remain hidden to conventional probes. Using X-ray total scattering and pair distribution function analysis, we uncover local symmetry breaking in structurally high-symmetry systems, revealing transient nanoscale states that strongly influence thermal transport. In chalcogenide thermoelectrics, this phenomenon—termed emphanisis—emerges upon warming as dynamic local distortions stabilized by configurational entropy, providing a microscopic origin of ultralow thermal conductivity [1,2]. Extending this concept, we show in SnSe that nanoscale symmetry breaking drives emergent dimensionality reduction, where atomic displacement correlations evolve from three-dimensional to quasi-two-dimensional within structural layers while becoming decoupled along the stacking direction [3]. This symmetry-broken state persists well above the phase transition and enhances phonon scattering, further suppressing heat transport. These results establish a unified framework in which hidden local distortions and reduced dimensionality act as fundamental mechanisms for thermal conductivity suppression, offering new strategies for designing high-performance thermoelectric and quantum materials.

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Room-Temperature Excitons and Exciton Dispersion in a Two-Dimensional Quantum Spin Hall Insulator

Armando Consiglio

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Abstract. Bismuthene (Bi:SiC), a monolayer of bismuth atoms grown on a silicon carbide substrate, is a prototypical two-dimensional quantum spin Hall insulator characterized by a large direct band gap at the K and K' valleys of the Brillouin zone. Its sizeable gap makes the system particularly suitable for investigating excitonic effects even under room-temperature conditions. Optical spectroscopy measurements, supported by ab initio *GW* and Bethe-Salpeter equation calculations, have revealed the presence of strongly bound excitons with considerable oscillator strength, providing evidence of excitons in a two-dimensional topological insulator. The excitonic properties of bismuthene arise from the interplay between strong Coulomb interactions, spin-orbit coupling, and nontrivial electronic topology. Besides the optical response at zero center-of-mass momentum, recent efforts have focused on the dispersion of excitonic states at finite momentum and on the resulting exciton band structure. These studies are motivated by theoretical developments on topological excitons. Understanding the exciton dispersion in Bi:SiC may provide insight into the geometric and topological properties of excitonic bands in two-dimensional topological materials.

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Fano Universality Revisited: Phonon Decoupling as a Pathway to Expedient Raman Spectral Analysis

Dejan M. Djokić[a], Dimitrije Stepanenko[a] and Marko Opačić[a]

[a]*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, Belgrade 11 080, Republic of Serbia*

Abstract. Fano resonances are a common spectral signature in Raman measurements of metals and doped semiconductors. However, their quantitative analysis has long relied on nonlinear fitting routines that are computationally expensive and offer limited physical transparency. In this presentation, we introduce a fitting framework grounded in an angular parametrization of renormalized Fano lineshapes, which reveals the intrinsic symmetries and spectral invariants encoded in their universal geometry. Key fitting targets, such as extremal separations and nodal points, are analytically linked to physically meaningful microscopic parameters, thereby bypassing the need for time-consuming numerical optimizations. The dimensionless Fano profile is further interpreted within a many-body framework as reflecting isolated dressed single-phonon dynamics with corrected Raman vertices, cleanly decoupled from purely electronic contributions. This decomposition directly informs the fitting strategy by reducing the effective parameter space and sharpening the physical interpretation of each fitted quantity. Validation against reported Raman data for doped silicon confirms that the approach substantially reduces computational complexity while maintaining full physical transparency.

Why are photonic qubits based on deterministic quantum light sources key to future quantum technologies and how can we engineer them for practical applications?

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Abstract. Quantum technologies are rapidly transitioning from fundamental research to real-world applications, with the potential to revolutionize computation, communication, and sensing. At the heart of this transformation lies the concept of the qubit - the fundamental unit of quantum information, which can be implemented across a variety of physical platforms, including superconducting circuits, trapped ions, and photonic systems. Each approach offers distinct advantages and limitations in terms of scalability, coherence, and operational complexity. Among these, photonic qubits stand out as particularly promising for quantum communication due to their robustness against environmental decoherence and their natural compatibility with existing optical fiber infrastructure. Photons offer multiple degrees of freedom for encoding quantum information, such as polarization, path, frequency, and time-bin encoding. While polarization encoding remains one of the most widely used approaches, it is highly sensitive to environmental perturbations and polarization drift in long-distance fiber communication. In contrast, time-bin encoding provides significantly improved robustness against decoherence during transmission through optical fibers, making it particularly attractive for long-distance quantum communication, scalable quantum networks, and practical quantum key distribution protocols. Owing to its intrinsic stability and compatibility with existing telecom infrastructure, time-bin encoding is increasingly regarded as one of the most promising routes toward real-world quantum cryptography systems. A key requirement for advancing photonic quantum technologies is the realization of efficient, stable, and scalable single-photon emitters (SPEs). Ideal SPEs must generate on-demand, high-purity photons with controllable properties while remaining compatible with integration into photonic and optoelectronic platforms. In this talk, I will present our recent work on III-nitride nanowire systems based on GaN/InGaN quantum-dot-like emitters, focusing on the demonstration of time-bin encoded single-photon emission as a proof of concept for future quantum communication technologies. By coupling these emitters to surface acoustic waves (SAWs), we achieve dynamic modulation of excitonic transitions at high frequencies, enabling controlled temporal manipulation of photon emission and the realization of time-bin photonic states. Although demonstrated in the InGaN material platform, the presented concept is not limited to III-nitride systems and can, in principle, be extended to a broad range of single-photon emitter platforms. This makes the approach particularly relevant for the wider development of scalable and application-ready quantum photonic technologies. The demonstrated dynamic control mechanism represents an important step toward robust fiber-compatible quantum light sources and practical implementations of secure quantum communication protocols.

Mechanism of Charge Transfer and Electrostatic Field Fluctuations in High-Entropy Metallic Alloys

Vladimir Dobrosavljevic [a]

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Abstract. High-entropy alloys present a new class of disordered metals which hold promising prospects for the next generation of materials and technology. However, much of the basic physics underlying these robust, multifunctional materials – and those of other, more generic forms of disordered matter – still remain the subject of ongoing inquiry. We here present a minimal-working model that describes the disorder-driven fluctuations in the electronic charge distributions and electrostatic "Madelung" fields in disordered metals. Our theory captures the leading contributions from dominant electronic processes, including electrostatic screening and impurity scattering events. We elaborate on the nature of these electronic charge and Madelung field fluctuations by determining how these emerge from the statistics of the underlying disorder, and how these can be described using the linear response formulation that we utilized. In doing so, our work answers various questions which have long-puzzled the disordered materials community. It opens up a path for obtaining systematic corrections to conventional first principles approaches to disorder-modeling (e.g. the standard KKR-CPA methods) at a computational cost much more modest than large-scale supercell methods such as LSMS.

Transport Through a Junction With a Precessing Anisotropic Molecular Spin

Milena Filipović

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Abstract. The subject of the study is charge transport through a molecular orbital connected to two Fermi leads and coupled to a precessing anisotropic molecular spin in a magnetic field, via exchange interaction.[1] The total precession frequency is modulated by the magnetic field and the uniaxial magnetic anisotropy parameter of the molecular spin. The expressions for the charge current and noise are derived by means of the Keldysh nonequilibrium Green's functions technique.[2] The inelastic tunneling processes between molecular quasienergy levels are driven by the molecular spin precession. The dc-bias voltages allow to reveal the quasienergy level structure, the anisotropy parameter, and the Larmor frequency through characteristics of transport measurements such as steps, peaks and dips. Quantum interference effects between states connected with spin-flip processes manifest themselves as peaks (maximums) and dips (minimums) in the shot noise, resembling Fano-like resonance profiles.[3] These effects are controlled by the Larmor frequency and the anisotropy parameter. Under zero-bias conditions the precession frequency decreases with the increase of the anisotropy parameter, or the precession direction is altered, and the shot noise is reduced. By proper adjustment of the anisotropy parameter, the precession frequency can be suppressed, leading to the vanishing of the shot noise. The results show that the anisotropic magnetic molecules can be used to control charge transport in molecular junctions via the magnetic anisotropy parameter.

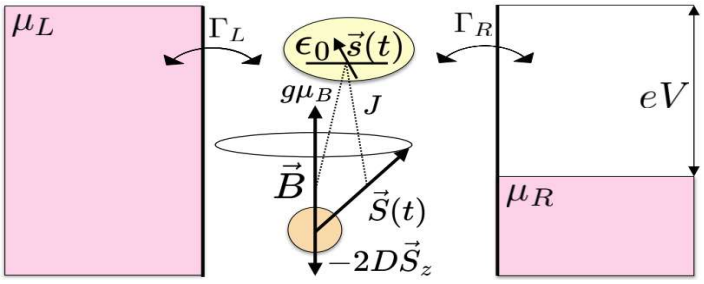

FIGURE 1. Tunneling through a single molecular orbital coupled to the anisotropic molecular spin in the presence of a magnetic field, connected to two Fermi leads. The spin of the molecule precesses around the magnetic field axis. Taken from [1].

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Hidden orders and polaron effectsin spin-orbit entangled correlated insulators

Cesare Franchini

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Abstract. In many materials, ordered phases and their associated order parameters can be readily identified using standard experimental probes. By contrast, *hidden order* denotes a phase transition in which thermodynamic signatures clearly indicate the emergence of an ordered state, while the underlying order parameter remains elusive to conventional characterization. The origin of such unconventional phases is often rooted in strong spin-orbit coupling, which entangles intersite exchange, electron correlations, and electron-phonon interactions. This intricate interplay makes hidden-order physics challenging to unravel, both experimentally and theoretically [1]. In this talk, I will discuss the emergence of hidden-order phases in correlated, spin–orbit-active osmium-based double perovskites, where ordering is governed by high-rank multipole moments [2,3]. I will then show how charge doping in Os double perovskites can drive *polaron formation*. These quasiparticles, arising from the coupling between excess charges and lattice vibrations [4], act as inhibitors of the Mott transition [5] and as mediators of hidden multipolar magnetic transitions [6]. Our theoretical predictions are supported by a variety of spectroscopic measurements.

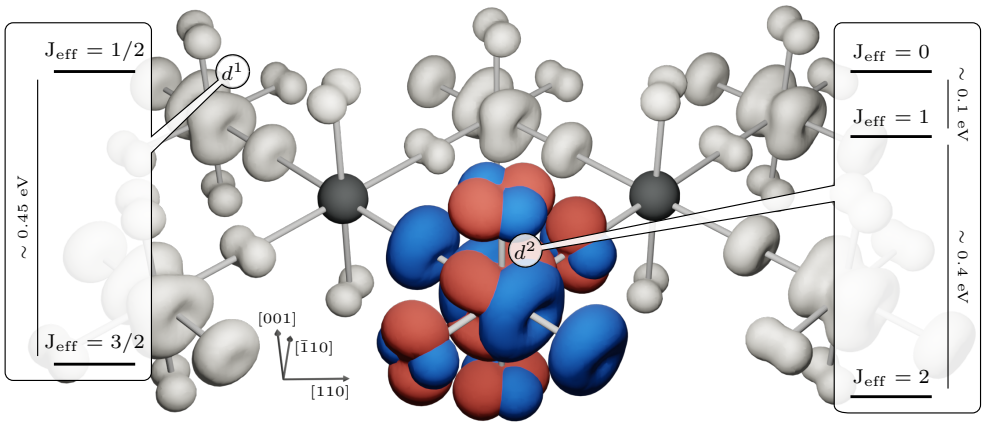

FIGURE 1. Hidden Bipolaron in a Spin-Orbit Correlated Insulator

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Light Scattering in Novel Quantum Materials

Rudi Hackl

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Abstract. Inelastic light (Raman) scattering is an important method for characterizing and studying materials [1]. In this contribution, I shall present a brief overview over the method, give a few technical details and discuss recent results in iron-based superconductors and materials have a kagome plane as the essential building element. For the superconductors I summarize recent results on gap spectroscopy and collective modes [2]. Time permitting, I discuss the interplay of Weyl electrons and phonons in $Co_3Sn_2S_2$ [3].

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Exotic Phase Transitions in Chromates with Mixed Valence

Masahiko Isobe

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Max Planck Institute for Solid State Research, Stuttgart, Germany

Abstract. Transition metal oxides have long been of interest because of their potential to exhibit intriguing phenomena in solid-state chemistry and physics. Among these, mixed-valent oxides are notable for their ability to demonstrate metallic conductivity and novel phenomena involving spin, charge, and orbital degrees of freedom. Here, we present two exotic phase transitions in mixed-valence chromium oxides. One is the charge disproportionation triggered by the Bi lone pair. The second is the metal-insulator transition without charge ordering. To synthesize both chromates, high-pressure synthesis is necessary. $BiCu_3Cr_4O_{12}$ has an *A-site-ordered* perovskite structure and is a mixed-valence oxide with $Cr^{+3.75}$. In $BiCu_3Cr_4O_{12}$, a ferrimagnetic transition with structural distortion was observed at ~ 185 K. The resistivity exhibits an anomaly at the transition, but metallic behavior persists even in the magnetic phase. We revealed charge disproportionation below the transition temperature through structural analysis. The origin of the transition is the local distortion of the BiO_{12} polyhedron for Bi 6*s*-O 2*p*-Bi 6*p* hybridization. The structural distortion stabilizes the Cr-O hybridization of the $Cr^{4+}O_6$ octahedra. As a result, the two types of $Cr^{3.5+}O_6$ and $Cr^{4+}O_6$ chains were ordered in a rocksalt-type substructure in the ac plane in the low-temperature phase. This is the first observation of the Bi-lone-pair-triggered charge disproportionation transition in mixed-valent chromium oxides [1]. Hollandite $K_2Cr_8O_{16}$ is a mixed-valence oxide with $Cr^{3.75+}$. $K_2Cr_8O_{16}$ is a ferromagnetic metal with T_C = 180 K, which is explained by the double-exchange mechanism. This ferromagnetic metal phase undergoes a transition to an insulator at T_{MI} = 95 K, while retaining its ferromagnetism [2]. In the low-temperature ferromagnetic insulator phase, there was no evidence of charge separation or order. However, we observed a slight structural distortion using synchrotron X-ray diffraction. In addition, detailed electronic structure calculations have demonstrated that the metal-insulator transition is caused by Peierls instability in a quasi-one-dimensional structure comprising four CrO_6 chains [3, 4]. We demonstrated that an uncommon ferromagnetic insulator phase can be realized in $K_2Cr_8O_{16}$ via a metal-insulator transition due to the Peierls mechanism in a system of fully spin-polarized electrons. However, a possible metal-insulator topological transition has recently been considered [5]. This metal-insulator transition is a rare and intriguing phenomenon that is still under discussion.

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Open Science in Serbia: Not a Fairy Tale, but a Good Case Study

Biljana Kosanović

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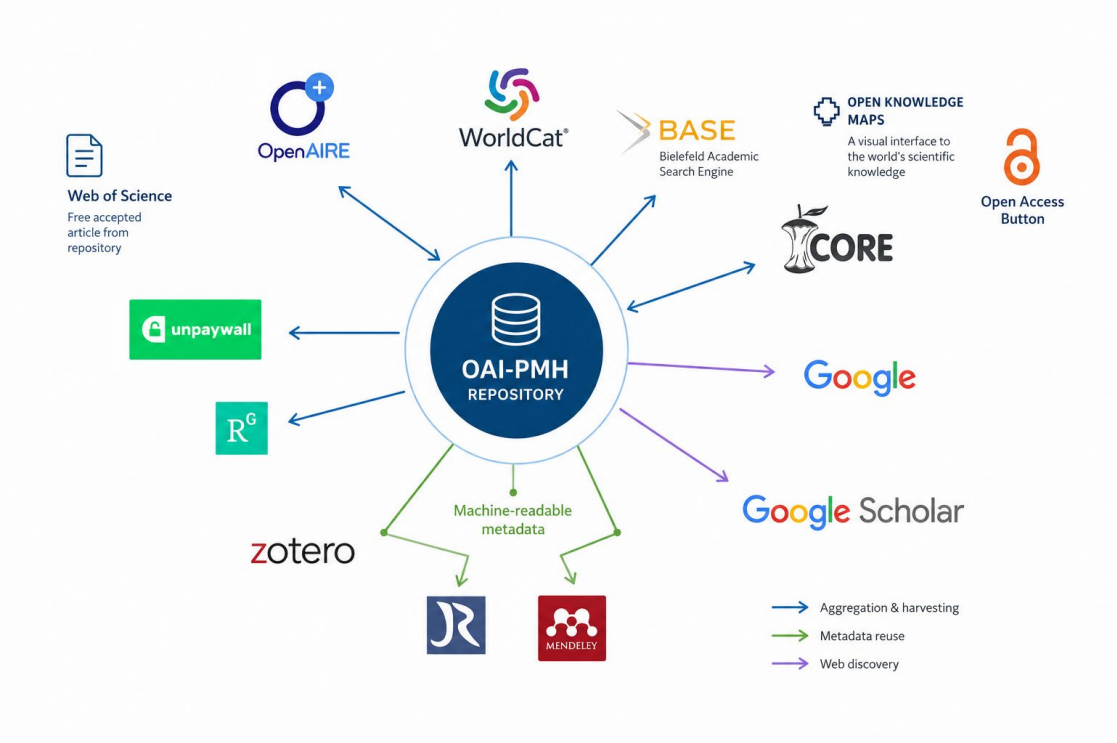
Abstract. Serbia has made significant progress in developing a national Open Science ecosystem during the last decade. A major milestone was the establishment of the national Open Science platform in 2018, followed by a new and upgraded version launched in 2024. The platform supports open access to scientific publications and increasingly addresses research data management and FAIR data principles, aiming to improve the visibility, accessibility, and reusability of publicly funded research results.

Alongside policy development, Serbia has invested in building the necessary infrastructure for Open Science. National repositories, journal platforms, persistent identifier systems, and interoperability services have been developed to support researchers, institutions, and publishers. These infrastructures enable better preservation, dissemination, and international integration of Serbian scientific output.

An important component of this ecosystem is education and capacity building. The University Library in Belgrade actively organizes training programs and workshops for young researchers, focusing on topics such as open access publishing, research data management, academic visibility, copyright, and responsible research practices.

Serbia is also part of the European Open Science landscape through its participation in OpenAIRE. Integration with OpenAIRE strengthens interoperability with European research infrastructures and supports the wider dissemination of Serbian research within the European Research Area.

FIGURE 1. Map of supporting infrastructure for Open Science in Serbia (Eco-system)



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Phonon Response of FeSe Under Uniaxial Strain

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Abstract. The interplay between lattice, charge, and spin degrees of freedom is crucial for understanding the physical behavior of correlated materials. In FeSe, symmetry-breaking perturbations offer a powerful approach for probing these interactions. Previous investigations have demonstrated that defects and isoelectronic substitution can significantly influence lattice–electronic coupling, frequently leading to the appearance of additional phonon-related features. In this work, uniaxial strain is utilized as a controllable symmetry-breaking parameter to examine the intrinsic lattice response of FeSe without introducing disorder.

The temperature dependence of phonon excitations was studied with high temperature resolution near the nemato-structural transition temperature Ts, with strain applied along the ⟨110⟩ and ⟨100⟩ crystallographic directions. In the absence of strain, the A_1g phonon mode exhibits a slight asymmetry within a narrow temperature range around Ts, suggesting the presence of an additional excitation in the fully symmetric Raman channel. When uniaxial strain is applied, this feature becomes considerably more pronounced.

The observed behavior is linked to fluctuation-driven changes in the coupling between lattice and electronic degrees of freedom above the nematic transition. Enhanced nematic fluctuations increase the likelihood of phonon-electron-phonon processes near the X and R points of the Brillouin zone, resulting in two-phonon scattering close to the A_1g mode. The intensity and observability of this scattering are strongly affected by both the magnitude and orientation of the applied strain, underlining the remarkable sensitivity of FeSe to local symmetry breaking.

Cost-Efficient Deterministic Engineering of Quantum Light Emitters in Two-Dimensional Semiconductors

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Abstract. Two-dimensional (2D) van der Waals semiconductors have emerged as a powerful platform for quantum photonic technologies due to their strong excitonic confinement, strain-tunable bandgaps, and compatibility with scalable nanophotonic architectures. In particular, localized excitonic states in layered materials such as GaSe and WSe_2 have recently demonstrated single-photon emission, positioning these systems as promising solid-state quantum light sources. However, a major bottleneck remains: how to achieve scalable, deterministic, and low-cost positioning of quantum light emitters.

Here, we present a lithography-free, cost-efficient, and highly reproducible strategy for the deterministic engineering of quantum light emitters in 2D semiconductors using optically active microparticles with a designed bipyramidal geometry. Mechanically exfoliated GaSe and WSe_2 flakes are transferred onto a Si/SiO_2 substrate pre-decorated with $LiYF_4:Nd^{3+}$ microparticles, whose sharp edges locally bend the 2D crystal, inducing nanoscale strain gradients that create quantum-confined excitonic traps. The optical activity of the microparticles (emission at 1.436 eV) provides a built-in, non-invasive reference that enables sub-micrometer localization of the strain-induced emitters using standard micro-photoluminescence, eliminating the need for atomic force microscopy or scanning electron microscopy [1]. Low-temperature μ-PL measurements reveal the emergence of narrow, spectrally isolated emission lines at the strain maxima, which are absent in unstrained regions of the flakes. Power-dependent and polarization-resolved spectroscopy identify these lines as exciton (X) and biexciton (XX) states originating from the same localized trap, exhibiting collinear elliptical polarization and a biexciton binding energy of ≈5 meV, corresponding to a confinement radius of ~13 nm. Crucially, photon-correlation measurements using a Hanbury Brown–Twiss interferometer demonstrate single-photon emission with $g^2(0) \approx 0.2$, which approaches zero after background correction, confirming the non-classical nature of the emission [1]. The observed X–XX cascade further indicates that these strain-engineered emitters are suitable for entangled photon-pair generation, a key requirement for quantum communication and photonic quantum information processing. Compared with state-of-the-art approaches based on e-beam lithography-defined nanopillars or focused-ion-beam nanostructures, our method offers an orders-of-magnitude reduction in cost and complexity while preserving emitter quality and spatial determinism.

Because the microparticles can be pre-patterned and oriented, this platform naturally lends itself to large-area arrays of site-controlled quantum emitters and is compatible with integration into on-chip photonic and acousto-optic architectures. This work establishes a scalable and accessible route to engineered quantum light in 2D materials, paving the way toward practical quantum photonic devices based on layered semiconductors.

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Spin Crystallographic Groups and Magnetic Arrangements in Low-Dimensional Structures

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Abstract. Symmetries of magnetic systems are tightly bound to the crystalline symmetries, and this observation is at the core of Shubnikov's theory of black-and-white magnetic groups. Magnetic arrangements assume that site spins are axial (pseudo) vectors subdued to magnetic groups, which are composed of geometrical transformations and their composition with time reversal. However, these groups are symmetries of magnetic systems with significant contribution of spin-orbit coupling, while the vast majority of complex but still symmetrical spin structures (such as helical and conical) cannot be described within this framework. Historically, studies on the Heisenberg Hamiltonian, which has more symmetry than it is required by the magnetic groups, had resulted in spin group formalism [1,2]. Spin groups are unavoidable tools for analyzing magnetic systems with neglected spin-orbit coupling, and for understanding the interplay of their symmetry and topology of their electronic/magnonic band structure, as well as for describing the altermagnets. Here, we focus on low-dimensional (in particular quasi-2D) magnetic systems and utilize an efficient algorithm [3] based on the irreducible representations of a crystallographic parent group to derive corresponding spin groups, and all related magnetic structures. As, in the group-theoretical language a spin group is defined as the product of a non-trivial spin group and spin only part [2], for a given parent group, we first derive the non-trivial part of a spin group. Then, for each Wyckoff position of the representative site, we determine the allowed representative spin vector in order to generate magnetic arrangement. The obtained arrangements are classified as linear, planar, and conical, and their symmetry is extended by the spin only group. We discuss the influence of the increased symmetry on pairwise spin Hamiltonian and magnon spectra, through the relation of magnetic and spin groups. These results complement the spin group database [2-6].

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Probing Green's Function Zeros by Co-tunneling through Mott Insulators

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Abstract. Quantum tunneling experiments have provided deep insights into basic excitations occurring as Green's function poles in the realm of complex quantum matter. However, strongly correlated quantum materials also allow for Green's functions zeros (GFZ) that may be seen as an antidote to the familiar poles, and have so far largely eluded direct experimental study. Here, we propose and investigate theoretically how co-tunneling through Mott insulators enables direct access to the shadow band structure of the GFZ, which characterize the Mott gap. In particular, we first derive an effective Hamiltonian for the GFZ that governs the low-energy behavior of the Green's function. We then demonstrate how the GFZ modifies the cotunneling amplitude, highlighting clear signatures of many-body correlations that distinguish the GFZ structure from the underlying free Bloch band structure of the system.

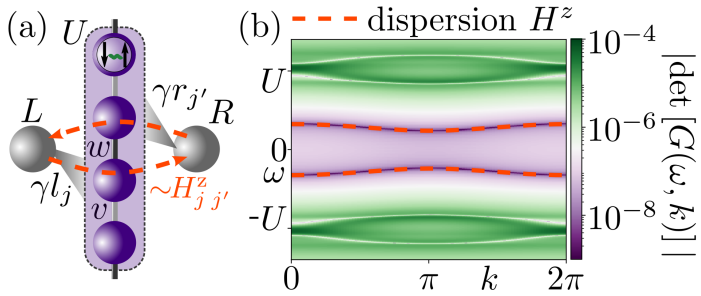

FIGURE 1. Co-tunneling reveals GFZ-Hamiltonian H^z: (a) Two spinful auxiliary sites (grey, $\{L,R\}$), weakly coupled by tunneling amplitudes $\{\gamma l_j, \gamma r_{j'}\}$ to a Hubbard system in Mott regime (violet). Elastic co-tunneling establishes an effective coupling between L and R (red, dashed line). (b) Numerical results (MPS, SSH-Hubbard model) on the GF-determinant $|\det[G(\omega,k)]|$ and analytic prediction of the in-gap zero dispersion of H^z (red, dashed line).

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Neutron Imaging at ILL: Expanding Capabilities for Operando and Multi-Scale Materials Characterisation

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Abstract. The Institut Laue-Langevin (ILL), Grenoble, is expanding its neutron imaging capabilities through the commissioning of several instruments, supported by the creation of the new Applied Science group, which integrates imaging, strain scanning, and irradiation platforms. The imaging instruments, along with the well-established NeXT, include the newly commissioned MoTo and PorTo instruments, and the upcoming high-flux thermal imaging station ThRILL. These are complemented by SALSA, the strain-scanning diffractometer, and TENIS, the material irradiation station. These developments establish a multi-instrument suite focused on advanced neutron characterisation across a range of disciplines, including materials science, energy and electrochemistry, metallurgy, manufacturing, as well as wide engineering applications. NeXT is a neutron and X-ray imaging platform supporting radiography and tomography together with advanced techniques, including Bragg-edge imaging, polarised imaging, grating interferometry, neutron laminography, with a newly integrated high-power X-ray source. The instrument has undergone upgrades over the years to enable complex *in-situ* experiments with the ability to host large-scale sample environments. MoTo, located adjacent to NeXT, employs a highly sensitive monochromatic cold beam for imaging, focusing on polarised neutron imaging and grating interferometry, enabling investigations of magnetic domains in material systems and microscale heterogeneities in complex metallic materials and alloys. PorTo, the newly commissioned micro-imaging neutron tomography station, focuses on high-resolution radiographic and tomographic imaging with the capability for laboratory-scale operando and in situ experiments. The instrument is designed to seamlessly enable higher-resolution three-dimensional studies of complex materials and dynamic processes. This contribution presents the capabilities of neutron imaging at ILL, with scientific highlights from NeXT and first scientific applications from MoTo and the commissioning phase of PorTo. Example applications range from tracking hydride formation in metallic materials and visualising local *in-situ* water dynamics in fuel cells, to studying two-phase flow and liquid water redistribution in porous transport layers, following liquid electrolyte redistribution in compact battery concepts, locating micro-defects in additively manufactured materials, studying moisture transport in porous media, and micro-imaging of small biological specimens. Particular emphasis is placed on the complementarity between imaging contrasts and modalities available across the instruments, and on the new scientific opportunities offered to the growing user community arising from combining neutron imaging with diffraction and irradiation methods within the Applied Science group.

Strain-Tunable Hysteresis of C-CDW and NC-CDW Transition in Bulk 1T-TaS_2

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Abstract. We investigate the influence of controlled uniaxial strain on the commensurate (C-CDW) to nearly commensurate (NC-CDW) phase transition in bulk 1T-TaS_2 using temperature-dependent Raman spectroscopy. Both compressive and tensile strain are applied, enabling a direct and symmetric comparison of their impact on phase stability and hysteresis.

The transition is tracked via characteristic Raman signatures of the C-CDW and NC-CDW states during both cooling and warming cycles. We observe clear first-order behavior with pronounced hysteresis. On cooling, the transition occurs reproducibly within a narrow temperature window (~150–160 K), indicating a relatively stable phase boundary. In contrast, the warming branch exhibits a broader strain-dependent transition (~160–180 K), consistent with metastability and history-dependent domain evolution. Strain-induced shifts of the transition temperatures, on the order of ~10 K, are resolved. Notably, the response is nearly symmetric for compressive and tensile strain, while the hysteresis width is reduced at larger strain amplitudes (±0.1%). The evolution of the warming transition suggests that strain influences the reorganization and mobility of domain-wall networks in the NC-CDW state.

Unraveling Material Evolution At The Nanoscale Via *In Situ* And *Ex Situ* Transmission Electron Microscopy

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Abstract. Nanostructured and nanoscale phases play a decisive role in the development of cutting-edge materials. Their unique properties, governed by increasing surface-to-volume ratio specific to nanoobjects, drastically affect the performance of the bulk material in which they are integrated, enabling tuning of its characteristics. Further advancement is barely possible without the comprehensive experimental analysis of the material evolution at the nanoscale. Transmission electron microscopy (TEM) stands out as an excellent tool for detailed material characterization, providing synergistic morphological, compositional, and crystallographic information. *In situ* TEM enhances this capability, enabling real-time observation of material changes under various stimuli, e.g., heating.[1,2]

Several case studies will be presented on how advanced TEM is employed to understand self-organization, phase formation, and decomposition at the nanoscale. First, the metal-semiconductor layered nanofilms will be discussed, representing a suitable model system for detailed real-time tracking of phase evolution via *in situ* TEM heating.[1] In particular, metal-induced crystallization, homogenization, and melting processes, as witnessed in a continuous experiment (Figure 1A), will be disclosed. The observed complex phase transformations and the components' solubility enhancement will be discussed within the framework of size effects in nanoscale systems. Then, it will be shown how the high-resolution TEM sheds light on the mechanism of resistive switching in the state-of-the-art phase change materials (PCMs), which are prominent for memristor applications (Figure 1B).[3]

The synergy of TEM approaches developed in this work establishes a solid basis for the planned project development with a particular focus on *in situ/operando* TEM investigation of nanoscale PCMs.

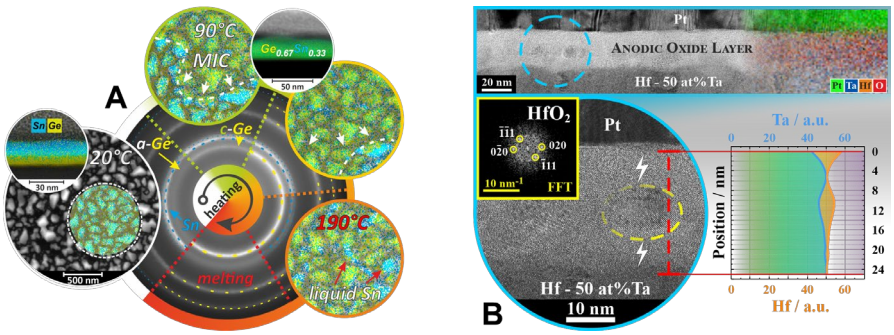

FIGURE 1. A - *in situ* TEM tracking the evolution of phases and their thermal stability in Ge–Sn nanofilms.[1] B - *post operando* TEM characterization of anodic Hf-Ta-based memristive material.[3]

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Diagrammatic Monte Carlo: exact solution of electron-phonon problem and a way to Kondo-Lattice enigma

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Abstract.

Bold Diagrammatic Monte Carlo (BDMC) is the Monte Carlo technique of self-consistent summation of the irreducible skeleton Feynman diagrams for the self-energy and polarization operator, which are used to modify (or boldify) the Green functions and interparticle interactions by solving the Dyson equation. Boldified diagrams and interaction propagators are used again to obtain the following step result for the self-energy and interaction, forming a self-consistent loop that often succeeds in circumventing the sign problem in many-body systems.

The BDMC was applied to a finite-density fermion gas with electron-phonon interactions [1, 2] and simultaneous electron-phonon and Coulomb interactions [3], showing the stability of the sign and demonstrating convergence even for strong couplings and low temperatures. This Real-Valued Green Functions (RVGF) method operates with real-valued electronic Green functions with a real chemical potential.

The BDMC was also applied to systems with interaction between localized spins (e.g., the Heisenberg model) [4, 5]. Since one cannot formulate diagrammatic techniques for spins because of their commutation relations, the Popov-Fedotov transformation [6] of spins into fermionic operators was used. The price for the luxury of having the Feynman diagrammatic technique for spins is the appearance of the imaginary chemical potential. However, the method of Complex-Valued Green Functions (CVGF) yields approximation-free results for real physical quantities, even in the case of frustrated magnetic systems.

The treatment of the Kondo effect requires the unification of the RVGF and CVGF approaches to describe both the itinerant and localised counterparts of the problem in the framework of the Fenman diagrammatic technique. We perform this unification and show the first preliminary results.

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Transport in electron-phonon systems: insights from the model systems

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Abstract. In clean, weakly doped semiconductors, electron transport is primarily limited by scattering with phonons. Key transport quantities, such as the frequency-dependent phonon mobility and diffusion constant, are traditionally calculated using the Boltzmann transport equation. However, beyond the regime of weak coupling and low temperatures, the foundational assumption of the Boltzmann approach—the existence of well-defined quasiparticles—begins to break down. This necessitates alternative approaches, such as the cumulant expansion method or the Migdal approximation (MA) combined with the independent particle approximation (IPA) within the Kubo formalism [1]. More sophisticated treatments include quantum Monte Carlo simulations or the self-consistent MA paired with either the IPA or the ladder approximation [2]. To evaluate the strengths and weaknesses of these methods, we examine them in well-controlled model systems where contributions to specific transport quantities can be isolated and calculated either numerically exactly or highly approximately [3,4,5]. By presenting results for the Holstein, Peierls, and Fröhlich models—representing three very different physical scenarios—we demonstrate that our conclusions are largely model-independent [6].

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Processing-Dependent Aging Behavior of Dental Resins: How Surface and Molecular Structure Dictate Color Stability and Translucency

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Abstract. This study comparatively evaluated the influence of processing routes on the optical stability of three dental resin composites: a light-cured direct composite—G-ænial A'CHORD (LCC), a CAD-CAM milled composite—BreCAM.HIPC (MC), and a 3Dprinted composite—Saremco Print Crowntec (PC). Specimens were analyzed before (T0) and after hydrothermal aging for 5000 (T1), 10,000 (T2), and 30,000 cycles (T3). Optical stability was assessed through the change in color (ΔE_{00}) and translucency parameter (TP) after aging and immersion in beverages. Surface topography was evaluated using atomic force microscopy (AFM), while Raman spectroscopy was employed to detect aging-induced molecular changes. After aging and staining, all composites exceeded the acceptability threshold for color change. ΔE_{00} values of 6.8 ± 1.1 (PC), 4.6 ± 0.9 (MC), and 2.1 ± 0.9 (LCC), obtained after initial aging, further increased following prolonged immersion in coffee. After 1 day of immersion in Coca-Cola, MC exhibited the highest ΔE_{00} values, which slightly exceeded the clinically acceptable threshold. Prolonged immersion (7 days) significantly increased staining for all materials. TP values significantly differed among materials, with the highest values detected for LCC (20.6 ± 3.6) and PC (19.1 ± 1.5) and the lowest values detected for MC (4.9 ± 0.8). Overall, the results demonstrated that ΔE_{00} was strongly influenced by the processing route and surface topography, whereas changes in translucency parameter (TP) were predominantly governed by the intrinsic properties of the resin composites.

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Breakdown of Drude transport and origin of c-axis resistivity maximum in layered oxides

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Abstract. We discuss the origin of c-axis resistivity maximum and associated non-metallic out-of-plane transport in layered oxides. Namely, in layered ruthenates, rhodates, cobaltates, …, the out-of-plane resistivity ceases to increase and starts to drop, whereas the in-plane resistivity continues to grow. This indicates that the Drude behavior, which tells that conductivity is proportional to the life time, cannot hold for both of them. We show that the Drude behavior breaks down for the case of out-of-plane transport when the corresponding velocities strongly depend on the in-plane momentum. This dependence leads to a certain energy scale and when the value of scattering exceeds this scale the resistivity ceases to grow with the scattering rate. We consider the Hund metal Sr_2RuO_4 as a test case, which we study within a realistic dynamical mean-field theory approach. The non-Drude behavior observed experimentally in c-axis transport is reproduced and explained by our considerations, showing that earlier invoked extrinsic mechanisms that involve either impurities or phonons are unnecessary.

Electron-phonon Decoupling in Kagome Lattice

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Abstract. Kagome materials have emerged as a fertile platform for exploring the connection between frustrated geometry and various interesting physical properties. Here, an overview of electron-phonon coupling in kagome and kagome-based systems composed of highly symmetric orbits is provided. The existence of electronic states at highly symmetric special points of the Brillouin zone that are completely decoupled from the ionic subsystem is demonstrated. Some of these decoupled states are degenerate, and for these, the Jahn-Teller theorem is violated. Finally, all kagome-based compounds composed of special orbits with decoupled states are identified.

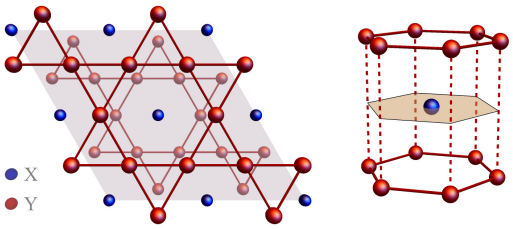

FIGURE 1. XY_3 Kagome system.

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Colossal magnetoresistance in insulating $EuCd_2As_2$

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Abstract. EuCd2As2, an A-type antiferromagnet with a Néel temperature of 9.5 K, has recently attracted considerable attention within the field of topological quantum materials. Initially proposed as an ideal Weyl semimetal, it was subsequently identified as a magnetic semiconductor with an energy gap of approximately 0.8 eV, as demonstrated by D. Santos-Cottin *et al.* in $EuCd_2As_2$: A Magnetic Semiconductor. Despite this revised classification, $EuCd_2As_2$ exhibits a remarkably rich spectrum of physical phenomena, including colossal magnetoresistance and an intrinsic spin-valve-like behavior. Moreover, its electronic properties can be effectively tuned via controlled modification of the carrier concentration.

In this talk, we present a systematic study of the magnetotransport properties of $EuCd_2As_2$ single crystals across the metal–insulator crossover induced by chemical tuning. We show that while both metallic and insulating regimes exhibit negative magnetoresistance, the magnitude differs dramatically: reaching nearly 10^6 in the insulating phase, compared to ~100% in the metallic state. In addition, the insulating regime displays an unconventional Hall response, in stark contrast to the conventional behavior observed in metallic samples, pointing to a fundamentally different transport mechanism. These results highlight the interplay between magnetism, electronic structure, and disorder in $EuCd_2As_2$, and establish it as a compelling system for exploring extreme magnetotransport phenomena in correlated magnetic semiconductors.

Andreev Bound State Spectra and Nonreciprocal Josephson current in SFFS Junctions with Interfacial SOC

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Abstract. We study nonreciprocal charge transport in planar two-dimensional Josephson junctions with arbitrarily oriented exchange fields in two ferromagnets within the barrier and interfacial Rashba spin–orbit coupling. The superconducting electrodes are assumed to have either *s*-wave or arbitrarily oriented *d*-wave order parameters. By performing a systematic symmetry analysis of the junction Hamiltonian, we identify the minimal conditions for the emergence of the anomalous Josephson effect and the Josephson diode effect, and classify the junctions into three distinct symmetry classes. These results are supported by numerical calculations of the current–phase relation within the Bogoliubov–de Gennes framework using a generalized Furusaki–Tsukada approach. We further examine how the orientation of spin-splitting fields in the two ferromagnets influences the phase-dependent Andreev bound state (ABS) spectrum and its signatures in nonreciprocal transport. Analysis of the phase-dependent ABS spectrum shows that, under conditions where bound states dominate transport, the current–phase relations obtained from the ABS approach closely match those derived from the Furusaki–Tsukada method, indicating a negligible contribution from continuum states. Deviations arise in the presence of zero-energy crossings in the bound state spectrum, which produce sawtooth-like current–phase relations, while the Furusaki–Tsukada results remain smooth. In *d*-wave junctions, the reduced or vanishing superconducting gap enhances the role of continuum states, which can become the dominant contribution to the supercurrent. The asymmetry of the spectrum under phase inversion directly reflects finite anomalous currents and unequal critical currents in opposite directions.

Our study identifies the conditions for achieving significant diode efficiency in Josephson devices through control of the superconducting electrode orientation and the direction of exchange fields in the ferromagnetic layers.

Zitterbewegung Chirality and Its Relation to Berry Curvature

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Abstract. Zitterbewegung, the trembling motion arising from interband quantum coherence, is a fundamental dynamical phenomenon originally introduced in relativistic quantum mechanics and later identified in a wide class of Dirac and Dirac-like condensed-matter systems. Previous studies have predominantly focused on its oscillatory character, emphasizing frequency, amplitude, and decay. However, an explicit connection between Zitterbewegung and band geometry has remained elusive. We establish an exact analytical relation between Zitterbewegung dynamics and Berry curvature in two-dimensional Dirac systems. By introducing a time-independent antisymmetric observable—the areal rate of Zitterbewegung—we show that it is directly controlled by the Berry curvature, with its sign fixing the chirality of the motion and reproducing the Dirac-point contributions to the Chern number. Remarkably, this relation is independent of the initial state and holds for generic two-band Dirac Hamiltonians.

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Polarons with Nonlinear Electron-Phonon Coupling via Diagrammatic Monte Carlo in Displacement Space

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Abstract.

Polaron physics plays a central role in understanding charge transport in materials with strong electron-phonon coupling, where electrons become dressed by lattice distortions to form quasiparticles with strongly renormalized properties. While the Holstein model provides a standard description based on harmonic phonons and linear coupling, this approximation breaks down in a growing class of materials, including quantum paraelectrics, hydrides, and halide perovskites, where lattice anharmonicity and nonlinear electron-phonon interactions are essential.

We study polarons with nonlinear electron-phonon coupling using a diagrammatic Monte Carlo approach formulated in the ionic displacement (X) representation [1, 2]. The method samples the perturbation expansion of the electronic imaginary-time Green's function with respect to electron hopping, providing an approximation-free framework that naturally incorporates arbitrary local lattice potentials, including strongly anharmonic double-well structures. It remains effective in the adiabatic regime, where conventional approaches often face severe limitations.

Using this approach, we compute ground-state polaron properties across different regimes and combinations of linear and nonlinear electron-phonon coupling. We focus in particular on the double-well regime, where we find that the non-monotonic dependence of the quasiparticle weight on quadratic coupling persists even in the deep adiabatic limit [2]. By extending the method to compute the imaginary-time current-current correlation function, we also extract signatures of the optical conductivity spectrum. These results highlight how nonlinear electron-phonon coupling fundamentally reshapes polaron dynamics in anharmonic materials.

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Effective Bands and Band-like Electron Transport in Amorphous Solids

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Abstract. The localization of electrons caused by atomic disorder is a well-known phenomenon. However, under which circumstances electrons remain delocalized and retain band-like characteristics even when the crystal structure is completely absent, as found in certain amorphous solids, is less well understood. To probe this phenomenon, we developed a fully first-principles description of the electronic structure and charge transport in amorphous materials, which combines a representation of the amorphous state as a composite (ensemble) of local environments and the state-of-the-art many-body electronic structure methods. Using amorphous In_2O_3 as an example, we demonstrate the accuracy of our approach in reproducing the band-like nature of the conduction electrons as well as their disorder-limited mobility. Our approach reveals the physical origins responsible for the electron delocalization and survival of the band dispersions despite the absence of long-range order.

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Stabilization of Single Atoms on 2D Materials: From Hydrogen Catalysis to Atomic-Scale Magnetism

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Abstract. Using computational methods based on density functional theory (DFT), we investigated the adsorption of metal atoms on two-dimensional (2D) materials, with a particular focus on strategies for stabilizing them as isolated single atoms. Such systems often exhibit electronic, catalytic, and magnetic properties substantially different from those of the corresponding bulk materials or close-packed clusters. The studied systems include metal atoms adsorbed on pristine and defected graphene and hexagonal boron nitride, demonstrating possible routes toward the realization of efficient single-atom catalysts for hydrogen recombination reactions [1,2]. Building on this, we further explored metal nanostructures formed on one-dimensional moiré graphene on nickel substrate, which exhibit highly anisotropic mobility and adsorption-site preferences governed by the electronegativity of the adsorbed metals [3]. Shifting the focus to magnetic phenomena at the atomic scale, we investigated holmium adatoms on ultrathin magnesium oxide films as representative single-atom magnets [4]. Similarly, we examined cobalt atoms embedded in the two-dimensional boron allotrope borophene [5], where the magnetic properties were analyzed by combining DFT calculations with the Heisenberg model.

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Ab initio Modelling and Computational Screening of Halide Perovskites & Ternary Halide Double Salts

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Abstract. Halide perovskites have revolutionized emerging photovoltaics and opto-electronics over the past decade, yet their computational modelling remains a rich and active field. In the first part of this talk, I will provide a brief introduction to the state of the art in first-principles modelling of key properties in these systems, including electron-phonon limited carrier mobilities and excitonic properties, and discuss the performance of hybrid functionals in capturing these phenomena accurately.[1-3] I will then transition to the second part, where the focus shifts from property modelling to materials exploration using ab initio calculations. Perovskite-inspired materials are emerging as a promising new class of candidates for both outdoor and indoor photovoltaic applications, owing to their favorable opto-electronic properties and reduced toxicity.[4] I will present our recent ab initio exploration of silver- and copper-based halide compounds, using the experimentally synthesized $AgBiI_4$ double salt as a structural prototype to investigate indium substitution as a route toward lead-free materials. By replacing Bi^{3+} with In^{3+}, we design the hypothetical compound $AgInI_4$ and assess its structural, electronic, and optical properties from first principles. Our calculations predict that $AgInI_4$ is both chemically and dynamically stable and exhibits a direct band gap of 1.72 eV, comparable to that of its bismuth analogue. However, its predicted photovoltaic performance is significantly reduced under both solar and LED illumination, as evaluated using the spectroscopic limited maximum efficiency metric. We show that this limitation stems from symmetry-forbidden optical transitions and from the absence of Bi-derived $6s^2$ lone-pair states at the valence band maximum — features that are crucial for the strong optical absorption observed in $AgBiI_4$. I will then present a high-throughput computational screening of the Ag–In–I ternary phase space, which reveals several stable and metastable compounds belonging to tetrahedrally and octahedrally coordinated structural families, with characteristic band gaps of approximately 3.0 eV and 2.0 eV, respectively. [5] Finally, I will broaden the discussion to our latest results spanning the Cu–In–I, Cu–Sb–I, Cu–Bi–I, and Ag–Sb–I phase spaces, offering a wider perspective on the stability and opto-electronic trends across copper- and silver-based halide materials.

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In Silico Discovery Of Novel Topological Materials

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Abstract. In my talk, I will present our efforts in data-intensive computational discovery of novel materials, in particular topological materials. We have developed a high-throughput computational screening methodology for identifying materials hosting various topological phases among known materials. The entire dataset of results from this high-throughput search is publicly available on the Materials Cloud platform [1]. Several predictions resulting from this search have been successfully confirmed by experiments. A new Z_2 topological insulator was theoretically predicted and experimentally confirmed in the β-phase of quasi-one-dimensional bismuth iodide Bi_4I_4 [2]. The electronic structure of β-Bi_4I_4, characterized by Z_2 invariants (1;110), is in proximity of both the weak TI phase (0;001) and the trivial insulator phase (0;000). We further predicted a robust type-II Weyl semimetal phase in transition metal diphosphides MoP_2 and WP_2, characterized by very large momentum-space separation between Weyl points of opposite chirality [3]. Recent experiments on WP2 revealed record magnitudes of magnetoresistance combined with very high conductivity and residual resistivity ratio [4], and many other extraordinary properties. I will discuss in detail the physical mechanism underlying magnetotransport in WP_2 as well as in other trivial and topological semimetals [5]. Finally, I will demonstrate that topological features in the band structures of common materials are indeed very common [6].

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The Serbian Reproducibility Network: Building Reliable and Open Research Practices in Serbia

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Abstract. Reproducibility and transparent research practices have become essential for scientific progress across disciplines, including solid-state physics and materials science. To support these developments at the national level, the Serbian Reproducibility Network (RS-RN) was established as a collaborative platform promoting open science, research integrity, and FAIR-aligned workflows.[1] The RS-RN brings together researchers, librarians, and infrastructure experts to strengthen methodological rigor and improve the reliability of scientific outputs within the Serbian research ecosystem. This talk presents the recent evolution of the RS-RN, highlighting its shift from initial coordination to active community engagement. Through national webinars, hands-on training, and thematic workshops covering topics such as transparent documentation, automated data extraction, and open research infrastructure, the network supports the adoption of reproducible methodologies across scientific fields. By aligning local practices with European and global standards, the RS-RN contributes to a broader cultural transformation toward openness, equity, and public trust in science. These efforts ensure that research results produced in Serbia become transparent, reusable, and well-positioned for international collaboration.

FIGURE 1. Serbian Reproducibility Network.

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Acknowledgements. The Serbian Reproducibility Network received seed money through the 'TIER2 Award for Establishing a Reproducibility Network'. TIER2 is funded by the European Union's Horizon Europe research and innovation programme under grant agreement No 101094817. The author acknowledges the Serbian Ministry of Science, Technological Development and Innovation (451-03-33/2026-03/200026) for support.

Experimental Evidence of Coherent-Like Phonon State in $InSiTe_3$

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Abstract. Layered van der Waals (vdW) materials are attracting a lot of attention due to their rich lattice dynamics and their potential to host a vast array of unique physical properties. The ternary telluride $InSiTe_3$ is a vdW material that has been relatively unexplored up until very recently.

In this work, we investigated the lattice dynamics of $InSiTe_3$ using polarization-resolved Raman spectroscopy. While the observed phonon modes are mostly consistent with the expected symmetry of the crystal structure, some deviations from conventional behavior are observed, such as additional spectral features emerging in specific polarization configurations, caused by an unusual self-organized coherent-like phonon state associated with a localized high energy A_g mode near 500 cm^{-1}. Temperature-dependent measurements reveal a non-monotonic evolution of observed phonon energies and linewidths, accompanied by the emergence of higher-order excitations at around 200 K. These effects point to strong phonon–phonon interactions, leading to the activation of multi-phonon scattering. Our results suggest that $InSiTe_3$ provides a promising platform for studying unconventional Raman responses driven by strong lattice interactions, offering insight into the interplay between symmetry, anharmonicity, and collective vibrational phenomena in low-dimensional materials.

Disorder And Electron–Phonon Coupling In 2H-$TaSe_{2-x}S_x$ Probed By Raman Spectroscopy

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Abstract. Charge-density-wave order in layered transition-metal dichalcogenides is highly sensitive to disorder, whereas superconductivity can survive once long-range CDW coherence is weakened. This behavior has been observed in several related systems, including disordered $NbSe_2$, $TiSe_2$-based compounds, and chemically substituted chalcogenides, where the balance between lattice coherence, electronic instability, and electron–phonon coupling shapes the resulting phase diagram. We investigate the alloy series 2H-$TaSe_{2-x}S_x$ ($0 \leq x \leq 2$), using Raman spectroscopy supported by density-functional theory calculations. Sulfur substitution introduces isoelectronic crystallographic disorder into a system where CDW order competes with superconductivity. The pristine end compounds show the expected first-order Raman-active phonons together with a broad two-phonon response, consistent with strong electron–phonon coupling. Alloying broadens the phonon lines and activates additional Raman features, consistent with disorder-induced relaxation of momentum selection rules and reduced translational coherence. Despite these disorder effects, the broad two-phonon structure persists across the full composition range, and the E_{2g}^2 phonon retains a pronounced Fano asymmetry. These signatures show that electron–phonon coupling remains robust even as the CDW state is suppressed. The results point to disorder-driven loss of long-range CDW coherence, rather than weakened electron–phonon coupling, as the dominant mechanism governing the evolution of 2H-$TaSe_{2-x}S_x$[1].

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Machine Learning The Order-Disorder Jahn-Teller Transition In $LaMnO_3$

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Abstract. We study the Jahn–Teller structural phase transition in $LaMnO_3$ at $T_{JT} \simeq 750$ K using molecular dynamics simulations driven by machine-learning force fields trained on ab initio data. Analysis of site–site correlation functions of the distortions shows that the transition is governed by the ordering of the Q_2 Jahn–Teller mode of the MnO_6 octahedra, which serves as the primary order parameter and indicates an order–disorder character of the transition. Notably, dynamic local distortions persist even above T_{JT}. Our simulations successfully reproduce the experimentally observed temperature dependence of both structural and phononic properties, emphasizing the role of anharmonic effects at finite temperatures. More generally, the combination of machine-learning-based molecular dynamics with velocity autocorrelation function analysis provides a powerful framework for elucidating the microscopic mechanisms of structural phase transitions in correlated materials. In particular, this approach enables a clear distinction between order–disorder and displacive transition mechanisms through the temperature evolution of vibrational behavior.

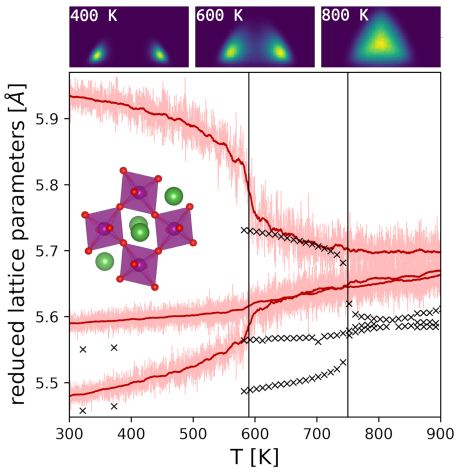

FIGURE 1. Jahn-Teller phase transition in $LaMnO_3$. The main panel shows the calculates lattice parameters (red lines) as a function of temperature compared to the exponential ones (crosses). The top panels show the distribution of MnO_3 octahedra in the (Q_2, Q_3) plane as a function of temperature.

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Diagrammatic Monte Carlo For Anisotropic And Degenerate Bands

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Abstract. The Diagrammatic Monte Carlo (DiagMC) technique has a well-established track record in the study of both large (Fröhlich) and small (Holstein) polarons [1]. Its main strength lies in its non-perturbative, all-coupling nature, allowing accurate treatment across the entire range of interaction strengths, unlike perturbative or variational approaches, which are generally confined to the weak- or strong-coupling limit, respectively.

That said, the Fröhlich and Holstein Hamiltonians rely on simplified assumptions: a single isotropic electron band with quadratic dispersion, a single optical phonon mode, and a simplified electron–phonon coupling. These assumptions often fail to capture the complex electronic and vibrational structures found in real materials. Extending DiagMC to realistic systems therefore requires going beyond these limitations. Recent progress has addressed this through the development of fully first-principles DiagMC frameworks [2], marking an important step forward.

In this work, we present DiagMC simulations of large polarons in real materials by relaxing the key assumptions of the original models. Using first-principles-based formulations [3], we compute several key quantities—energy renormalization, polaron effective masses, dispersion relations, and quasiparticle weights for a range of materials, including AlAs, BaO and CaO. We also benchmark our DiagMC results against existing studies [2,3,4], and especially the Feynman variational approach, finding good consistency and demonstrating the predictive power of the method.

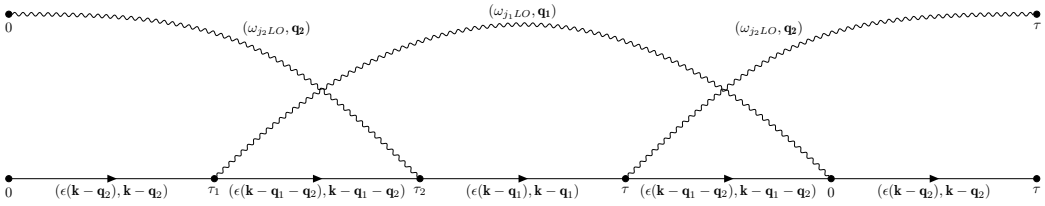

FIGURE 1. Diagram generated by DiagMC method.

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Electronic Properties of Layered Phyllosilicates: A First-Principle Analysis

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Abstract. Layered phyllosilicates, including talc and kaolinite-type minerals, constitute a class of naturally occurring materials whose structural characteristics closely resemble those of two-dimensional (2D) systems. Their layered architecture, defined by strong in-plane bonding and weaker interlayer interactions, makes them attractive platforms for studying low-dimensional behavior in naturally occurring compounds.
Structurally, phyllosilicates are composed of tetrahedral (T) sheets formed by SiO_4 units and octahedral (O) sheets containing metal-centered octahedra. In kaolinite-type minerals, layers adopt a 1:1 (T–O) configuration, whereas talc exhibits a 2:1 (T–O–T) structure, in which an octahedral sheet is enclosed between two tetrahedral sheets [1]. These distinct stacking arrangements not only define the layer geometry but also determine the nature of interlayer bonding mechanisms and the degree of coupling between adjacent layers.
In this study, we examine the electronic properties of layered phyllosilicates, with particular emphasis on talc and kaolinite-type systems. The calculated electronic band structures reveal wide band gaps within the PBE approximation, alongside a pronounced dependence of band dispersion on the layered crystal architecture. The differences observed between talc and kaolinite-type minerals originate from their distinct stacking arrangements and interlayer interactions, which directly influence electronic anisotropy and interlayer coupling.
The calculations were performed within the framework of density functional theory using the Quantum ESPRESSO package [2]. A plane-wave basis set combined with ultrasoft pseudopotentials was employed, with exchange–correlation effects described by the PBE generalized gradient approximation. Grimme-D2 van der Waals corrections were included to account for weak interlayer interactions.
Overall, these results provide fundamental insight into the relationship between crystal structure and electronic behavior in naturally occurring layered silicates. The presence of intrinsic two-dimensional building blocks, combined with structural diversity and tunable electronic characteristics through defects, doping, or layer engineering, make talc and kaolinite-type minerals promising candidates for use in van der Waals heterostructures, dielectric layers, and as substrates for two-dimensional electronic and optoelectronic systems. More broadly, these materials represent a versatile platform for exploring structure–property relationships in low-dimensional materials.

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Spectroscopic and Structural Characterization of Co(III), Cu(II), and Ni(II) Complexes with the Bioactive Hp_2DAP Ligand

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Abstract. Hydrazone-based Schiff bases are versatile ligands with strong metal-chelating ability and relevance in coordination and bioinorganic chemistry [1–2]. In this study, coordination compounds of the pentadentate N_5 donor ligand bis(3-chloropyridazine-6-hydrazone)-2,6-diacetylpyridine (Hp_2DAP) with Co(III), Cu(II), and Ni(II) ions [3] were synthesized and investigated using a multi-technique analytical approach, combining diffuse reflectance UV–Vis, Raman and FTIR spectroscopy, X-ray diffraction (XRD), and SEM–EDX.

Diffuse reflectance UV–Vis spectroscopy enabled reliable resolution of electronic transitions in the solid state. The Co(III) complex exhibits intense ligand-to-metal charge transfer bands characteristic of a μ-peroxo-bridged dinuclear structure. The Cu(II) complex shows a broad d–d absorption envelope (500–1000 nm) with multiple components, providing clear evidence of Jahn–Teller distortion in a tetragonally elongated d^9 system [4]. In contrast, the Ni(II) complex displays well-resolved d–d transitions consistent with a square planar d^8 geometry, indicating a rigid and conjugated ligand field. Raman spectroscopy confirms these findings, with a diagnostic O–O stretching mode (~810 cm^{-1}) in the Co(III) complex [5] and clear splitting of Cu–ligand vibrations supporting Jahn–Teller distortion. FTIR analysis revealed consistent coordination behavior across all complexes, confirming ligand binding through azomethine nitrogen atoms. This is evidenced by the absence of N–H stretching bands, the downshift of C=N vibrations, and the absence of carbonyl (C=O) bands, indicating complete ligand transformation and double deprotonation. Additional low-frequency bands confirmed the formation of metal–ligand bonds. XRD and SEM–EDX analyses reveal metal-dependent structural organization, ranging from amorphous Co(III) to moderately crystalline Cu(II) and highly crystalline Ni(II) systems.

Collectively, these results establish clear correlations between electronic structure, vibrational properties, and solid-state organization, providing a comprehensive framework for understanding the potential biological relevance of these complexes.

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Evolution Of Electron-Phonon Coupling Across A Topological Phase Transition In $ZrTe_5$

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Abstract. Since the experimental discovery of Dirac and Weyl semimetals and their unique electronic properties, including ultrahigh mobility, large magnetoresistance, chiral anomaly-induced transport, and topological surface states, considerable attention has been directed toward materials hosting closely related topological phases [1]. Among them, $ZrTe_5$, which lies near the boundary between strong and weak topological insulating phases, is a representative material [2]. It crystallizes in the orthorhombic *Cmcm* space group and adopts a layered structure composed of prismatic $ZrTe_3$ chains running along the *a* axis, interconnected by Te atoms within quasi-two-dimensional sheets, which are stacked along the *b* axis via van der Waals interactions [3]. This structural anisotropy is accompanied by a temperature-dependent band gap and electronic properties highly sensitive to lattice dynamics, with the electronic structure characterized by a nearly gapped Dirac-like dispersion [4,5]. Here, we present a temperature-dependent Raman study of Dirac semimetal $ZrTe_5$ single crystals in parallel and cross polarization configurations from 40-300 K. The study reveals anomalies in energy and linewidth across the Lifshitz transition for all detected symmetry-resolved phonons, as well as changes in the Fano asymmetry parameter for most A_g modes and both B_{2g} modes. Additionally, non-monotonic changes in energy, linewidth, and Fano asymmetry are observed in the 180-200 K range, coinciding with the temperature T_{AHE} associated with the emergence of the anomalous Hall effect.

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Interband Cascade Lasers With Hybrid Superlattice Plasmon-Enhanced Claddings For Operation Beyond The "Sweet Spot" Wavelength Range

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Abstract. We present interband cascade lasers (ICLs) with hybrid claddings, emitting at 5.2 µm. The wavelength matches the spectral line of nitrous oxide (NO), making it suitable for portable gas sensing application. The model of 8-stage GaSb-based ICL with hybrid claddings composed of outer plasmon-enhanced $InAs_{0.915}Sb_{0.085}$ and inner InAs/AlSb superlattice claddings is contrasted to the ICL of the same active region and geometry, but with purely superlattice InAs/AlSb claddings. Figure 1 presents the optical mode profiles of the two ICL structures. For the hybrid cladding structure, the mode gets more localized to the active region as the confinement factor is 11.2 % higher. This is a consequence of a significantly lower refractive index of plasmon-enhanced claddings. Figure 2 depicts the obtained threshold current density is $242\ A/cm^2$ in pulsed operation at room temperature. This is the lowest value reported to date for ICLs emitting at wavelengths longer than 5 µm. We also report close to record value threshold power density of $840\ W/cm^2$. Figures 3 (a) and 3 (b) show the spectra measurements of the narrow ridge waveguide ICL. The temperature series was measured in pulsed, whereas bias current series was measured in continuous wave (cw) operation. The extracted thermal resistance, as low as 62 K/W highlights improved heat dissipation of the ICL, which validates a high thermal conductivity of plasmon-enhanced claddings.

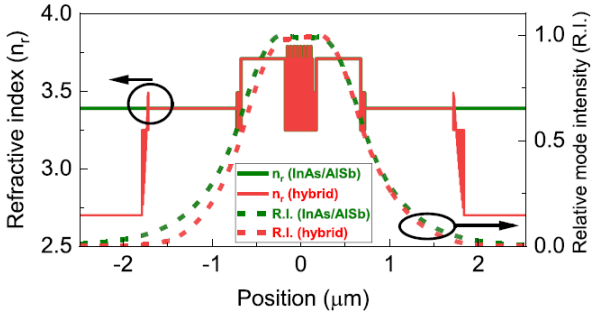

FIGURE 1. Refractive index profiles and optical mode intensities along the growt hdirection of two ICLs with the same separate confinement layers (SCLs) and active region design, but different cladding designs: standard InAs/AlSb superlattice claddings (green) and hybrid InAs/AlSb/InAsSb plasmon-enhanced claddings (red).

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