BOOK OF ABSTRACTS

ADVANCES
IN SOLID STATE PHYSICS
AND NEW MATERIALS

ДОСТИГНУЋА У ФИЗИЦИ ЧВРСТОГ СТАЊА И НОВИХ МАТЕРИЈАЛА

30 година Центра за физику чврстог стања и нове материјале Института за физику у Београду

ADVANCES IN SOLID STATE PHYSICS AND NEW MATERIALS

30 years of the Center for Solid State Physics and New Materials at the Institute of Physics Belgrade

19 - 23 May 2025
Belgrade, Serbia

Conference Chairs

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Emil S. Božin, *Institute of Physics Belgrade, Serbia*

Rudi Hackl, *IFW Dresden, Germany*

Zoran V. Popović, *Serbian Academy of Sciences and Arts (SANU), Serbia* – honorary chair

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Advances in Solid State Physics and New Materials

The international conference **"Advances in Solid State Physics and New Materials"** is being organized to celebrate the 30th anniversary of the **Center for Solid State Physics and New Materials** at the **Institute of Physics Belgrade (IPB)**. The conference, subtitled **"30 Years of the Center for Solid State Physics and New Materials at the Institute of Physics Belgrade"**, will take place from **May 19–23, 2025**, as a joint endeavor of the **Department of Natural Sciences of the Serbian Academy of Sciences and Arts (OTN SANU)** and the **Center for Solid State Physics and New Materials, IPB**.
The event commemorates the founding of the Center on May 24, 1995, and highlights its recognition as one of the first centers of excellence in nanoscience and nanotechnology in Serbia. The Center has also been acknowledged as a European center of exceptional value for applications of optical spectroscopy in physics, materials science, and environmental protection (OPSA). The conference is also part of the activities of the **HIP-2D-QM project**, conducted under the Horizon ERA Chair call, independently executed by researchers at the Center.

The program will cover a broad spectrum of topics in solid-state physics, including:

- New quantum materials
- Strong correlations
- Ordering phenomena and phase transitions
- 2D materials
- Topology
- Magnetism
- Unconventional superconductivity
- Semiconductors

Conference venue:
Serbian Academy of Sciences and Arts (SANU), Knez Mihailova 35, 11000 Belgrade, Serbia
Conference website: https://www.advances25.solidstate.ipb.ac.rs/

Advances in Solid State Physics and New Materials 2025 is organized by Center for Solid State Physics and New Materials at the Institute of Physics Belgrade (http://solidstate.ipb.ac.rs/) and Serbian Academy of Sciences and Arts (http://www.sanu.ac.rs/). Advances 2025 is organized with support of European Union's Horizon Europe research and innovation programme (https://research-and-innovation.ec.europa.eu/) under grant agreement No. 101185375 and Science Fund of the Republic of Serbia (https://fondzanauku.gov.rs/).

Funded by the
European Union

The support of the sponsors of Advances in Solid State Physics and New Materials 2025 is gratefully acknowledged:

Workshop 1: Quantum Phases and Ordering

Workshop Chair: Ana Milosavljević[a]

[a]*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118,11080 Belgrade-Zemun, Serbia*

The workshop Quantum Phases and Ordering explores the rich and diverse landscape of strongly correlated materials, focusing on emergent quantum phases and ordering phenomena. As part of the DYNAMIQS project (Dynamics of CDW Transition in Strained Quasi-1D Systems), funded by the Science Fund of the Republic of Serbia, these sessions bring together researchers investigating charge density waves, unconventional superconductivity, and topological or metastable quantum states. The program includes both experimental and theoretical contributions, addressing quantum criticality, symmetry breaking, ultrafast dynamics, and the interplay between electronic and lattice degrees of freedom. Special emphasis is placed on the effects of strain and reduced dimensionality in tuning and stabilizing novel phases. The workshop aims to foster discussion on how these intertwined factors drive complex behavior in correlated quantum systems.

Acknowledgement. This research was supported by the Science Fund of the Republic of Serbia through the PROMIS 2023 Research Program, Grant No. 10925, Dynamics of CDW transition in strained quasi-1D systems - DYNAMIQS

Project: *Dynamics of CDW Transition in Strained Quasi-1D Systems*

Acronym: DYNAMIQS

Grant number: **10925**

Funding: Science Fund of the Republic of Serbia - **Promis 2023 Program**

Workshop 2: Advanced Materials in Cultural Heritage Protection

Workshop Chair: Tijana Tomašević Ilić[a]

[a]*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade-Zemun, Serbia*

The workshop *Advanced Materials in Cultural Heritage Protection* adopts a multidisciplinary approach that integrates emerging technologies and their applications in the conservation and preservation of cultural heritage. It is organized by the 2DHeriPro project, funded by the Science Fund of the Republic of Serbia under the PRISMA program. The workshop objective is to bring together experts from diverse scientific fields to present their research on the condition and degradation of various artifacts, the necessity of conservation and restoration, potential challenges, and the application of novel materials and methods in conservation. The workshop also serves as a platform for the exchange of ideas and the fostering of collaborations on innovative approaches. As part of the program, a live demonstration will be held at the Faculty of Applied Arts, featuring analytical methodologies employed by scientists and conservators for the in situ study of historical artifacts. This demonstration will introduce participants to key tools and techniques for on-site analysis in archaeometry, conservation science, and cultural heritage preservation.

Acknowledgment: The organization of the workshop was supported by the Science Fund of the Republic of Serbia, Grant No 7456, 2D Material-based Tiled Network Films for Heritage Protection-2DHeriPro.

Workshop 3: Bioaerosols and nanoaerosols: interdisciplinary approaches in microbiology

Workshop Chairs: Predrag Kolarž [a] and Irena Aranđelović [b]

[a] *Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade-Zemun, Serbia*
[b] *Institute of Microbiology and Immunology, Faculty of Medicine, University of Belgrade, Pasterova 2, 11000 Belgrade, Serbia*

The workshop "Bioaerosols and nanoaerosols: interdisciplinary approaches in microbiology" presents the methodology, part of the results, and expected impacts of the project IonCleanTech, investigating the removal of microorganisms and other polluting particles from the indoor air by ionization. Indoor air pollution is considered to be one of the major threats to the public health. Bioaerosols include fungi, bacteria, archaea, viruses, allergens, toxins, and resistance genes – not only that they cause rapid spread of respiratory infections, but also trigger chronic diseases and other health problems. Other forms of air pollution and climate changes are both in favor of increased air transmission of bioaerosols. The IonCleanTech project strives to define optimized conditions for pollutant removal by directed streams of small air ions, and to develop products which efficiently deliver the ions, in appropriate concentrations and with optimal polarity ratios, to the breathing zone. The project is led by the Institute of Physics Belgrade and carried out in collaboration with the Faculty of Medicine and Faculty of Veterinary Medicine of the University of Belgrade.

Acknowledgement. This work resulted from and was financially supported by the Science Fund of the Republic of Serbia through the Green Program of Cooperation between Science and Industry (Project No: 5661, Project acronym: IonCleanTech).

Project: Elimination of respirable airborne particles, microplastics, microorganisms, and VOCs by ionization of indoor air and filtration systems: comprehensive investigation for reliable technological answers

IonCleanTech
Cleaner Air - Brighter Future

Acronym: IonCleanTech

Grant number: 5661

Funding: Serbian Science Fund - **Green Program of Cooperation between Science and Industry**

Workshop 4: Computational Analysis and Modeling of Biological Materials

Workshop Chairs: Anđelija Ilić[a] and Tijana Štajner[b]

[a]*Institute of Physics Belgrade, National Institute of Republic of Serbia, University of Belgrade, Pregrevica 118, 11080 Belgrade-Zemun, Serbia*
[b]*National Reference Laboratory for Toxoplasmosis, Group for Microbiology and Parasitology, Centre of Excellence for Food- and Vector-borne Zoonoses, Institute for Medical Research, National Institute of Republic of Serbia, University of Belgrade, Belgrade, Serbia*

The workshop "Computational analysis and modeling of biological materials" presents the underlying motivation, innovative approaches, and first year results of the project ToxoReTREAT, striving to improve the diagnostics and treatment options for reactivated toxoplasmosis. The project, led by the National Reference Laboratory for Toxoplasmosis, Institute for Medical Research, is a collaboration of four institutions including the Institute of Physics Belgrade. It combines advanced experimental work leading to the highest quality data with computational approaches used for the development of new drug candidates, as well as the analysis and quantitative assessments based on experimentally obtained digital images.

Acknowledgement. This work resulted from and was financially supported by the Science Fund of the Republic of Serbia through the PRIZMA Research Program (Project No: 7328, Project acronym: ToxoReTREAT).

Workshop 5: Research Opportunities at Large Scale User Facilities

Workshop Chairs: Emil S. Bozin[a] and Dušan Božanić[b]

[a]*Center for Solid State Physics and New Materials, Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*
[b]*Department of Radiation Chemistry and Physics, Institute of Nuclear Sciences "Vinča", University of Belgrade, Mike Petrovića-Alasa 12-14, 11351 Vinča, Belgrade, Serbia*

The workshop targets wide research audience in Serbia engaged in solid state physics, solid state chemistry, surface and materials science, atomic, molecular and optical physics, nanosciences and biomedical science with aims to highlight research opportunities at large scale user facilities (LSUF) in Europe and exemplify the LSUF research culture. The workshop will gather leading experts from large-scale facilities to facilitate knowledge exchange and promote cutting-edge experiments using advanced synchrotron-based photon and neutron sources. This workshop is synergistically organized by "Hidden Phases in Two-Dimensional Quantum Materials" (HIP-2D-QM) ERA Chair project, sponsored by the European Union's Horizon Europe research and innovation programme under grant agreement No 101185375, and ESUO – Serbia, the Serbian branch of the European Synchrotron and FEL user organization (ESUO).

ADVANCES IN SOLID STATE PHYSICS AND NEW MATERIALS

30 years of the Center for Solid State Physics and New Materials at the Institute of Physics Belgrade

CONFERENCE PROGRAM

LOCATION:
Serbian Academy of Sciences and Arts,
Kneza Mihaila 35, 11 000 Belgrade, Serbia

MAY 19–23, 2025
SERBIAN ACADEMY OF SCIENCES AND ARTS AND INSTITUTE OF PHYSICS BELGRADE

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 19	Session B – Hall 1	Time
08:30–09:30	**Registration**			**08:30–09:30**
09:30–10:30	**Opening ceremony**			**09:30–10:30**
10:30–10:50	**Coffee Break**			**10:30–10:50**
Chair	**Nenad Lazarević**		**Bojan Stojadinović**	**Chair**
10:50–11:20	**Thomas Devereaux** (USA) *"Thermal Hall in Quantum Antiferromagnets"*		**Nandakumar Kalarikkal** (India) *"Novel 2D Hybrid Platforms for Emerging Applications"*	**10:50–11:20**
11:20–11:50	**Kurt Hingerl** (Austria) *"Optical Transitions Between Entangled Electron-Phonon States"*		**Jasmina Lazarević** (Serbia) *"Exploring Structural Phase Transitions in Atorvastatin Calcium Trihydrate through Variable-Temperature Raman Spectroscopy"*	**11:20–11:40**
11:50–12:20	**Cedomir Petrovic** (China and Serbia) *"Fermi Surface characteristics in FeP_2"*		**Marko Opačić** (Serbia) *"Strain-dependent vibrational properties of $SrIrO_3$ thin films"* **Andrijana Šolajić** (Serbia) *"Strain Engineering in hBN/$M^{III}X^{VI}$ Heterostructures for Enhanced Optoelectronic Performance"*	**11:40-12:00** **12:00–12:20**
12:20–14:15	**Lunch Break**			**12:20–14:15**
Chair	**Thomas Devereaux**		**Zorica Popović**	**Chair**
14:15–14:45	**Milorad Milošević** (Belgium) *"Brain inspired computing with superconducting neurons"*		**Danica Krstovska** (N. Macedonia) *"Physical characterization and device application of organic bilayer films"*	**14:15–14:45**
14:45–15:15	**Leonardo Degiorgi** (ETH Zurich) *"Optical Signature of Anomalous Hall Effect in a Correlated Magnetic Weyl Semimetal"*		**Miroslav Požek** (Croatia) *"Phase Separation in Lightly Doped $La_{2-x}Sr_xCuO_4$ Studied by Cu NMR"*	**14:45–15:15**
15:15–15:45	**Vladimir Damljanović** (Serbia) *"Group-Theoretical Study of Simple Bands in Two-Dimensional Materials"*		**Božidar Šoškić** (Montenegro & Belgium) *"Superconducting Properties of Borophenes from First Principles "*	**15:15–15:45**
15:45–16:05	**Coffee Break**			**15:45–16:05**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 19	Session B – Hall 1	Time
Chair	**Milorad Milošević**		**Zorica Konstantinović**	**Chair**
16:05–16:35	**Jochen Geck** (Germany) *"Elastic lattice tuning and magnetic interactions of Kitaev materials" (online)*		**Zorica Lazarević** (Serbia) *"Innovative Approach to Studying the Structural, Magnetic and Electrical Characteristics of Nano Spinel Ferrites Prepared via Soft Mechanochemical Synthesis"*	**16:05–16:35**
16:35–17:05	**Zurab Guguchia** (Switzerland) *"Unconventional Superconductivity and Charge Order in Kagome Lattices Revealed by Muon Spin Rotation" (online)*		**Radoš Gajić** (Serbia) *"Wettability of Covellite"*	**16:35–17:05**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 20	Session B – Hall 1	Time
Chair	**Ana Milosavljević (WS1)**		**Matthias Opel**	**Chair**
09:00–09:30	**Andres Cantarero** (Spain) *„Thickness dependence of the CrI_3 dielectric function"*		**Marko Kralj** (Croatia) *"Exploring New Horizons: Epitaxial Growth of Next-Generation 2D Materials"*	**09:00–09:30**
09:30–10:00	**Hermann Suderow** (Spain) "Surface Charge Density Wave in UTe_2"		**Luka Pirker** (Czech Republic) *"The Role of Metallic Substrates in Large-Area Exfoliation of TMDCs"*	**09:30–10:00**
10:00–10:30	**Yann Gallais** (France) *"Ultrafast Raman scattering in quantum materials"*		**Antonio Bianconi** (Italy) *"Artificial High Tc SCs with Tc amplification on demand made of nano HSs by quantum design tuned at a Fano-Feshbach shape resonance"*	**10:00–10:30**
10:30–10:50	**Coffee Break**			
	Yann Gallais (WS1)		**Ivana Milošević**	
10:50–11:20	**Caitlin O'Neil** (Germany) *"The stress-strain relationship of quantum materials: New method developments and application to Sr_2RuO_4"*		**Igor Pašti** (Serbia) *"Unraveling the Electrochromic Mechanism of Ni-Deficient NiO: A Charge Localization Perspective from DFT+U Calculations"*	**10:50–11:20**
			Dimitrije Stepanenko (Serbia) *"Photon Condensation and Electromagnetic Response in Single Molecule Antiferromagnets with Flux Coupling"*	**11:20–11:40**
11:20–11:50	**Goran Karapetrov** (USA) *"Coexistence of Superconductivity and Chiral Charge Density Wave in $TiSe_2$"*		**Dejan Djokic** (Serbia) *"Unlocking the Universality of Fano's Effect in Raman Spectroscopy and Its Role in Condensed Matter Physics"*	**11:40-12:00**
11:50–12:20	**Zhenzhong Shi** (China) *"Elasticity of Charge Density Wave Superlattice in Low-dimensional Materials"*		**Anđelija Ilic** (Serbia) *"Applications of Small Air Ions and Electromagnetic Fields in Research with Biological Materials"*	**12:00–12:20**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 20	Session B – Hall 1	Time
12:20–14:15		**Lunch Break**		**12:20–14:15**
Chair	**Marko Kralj**		**Jelena Pešić**	**Chair**
14:15–14:45	**Matthias Opel** (Germany) *"Magnon Spin Transport in Antiferromagnetic Insulators"*		**Radmila Panajotovic** (Serbia) *"Graphene-based Composite Thin Films with Self Assembling Biomolecules as Active Elements in Sensors"*	**14:15–14:45**
			Ivana Milošević (Serbia) *"Tuning the Properties of Liquid-Phase Exfoliated Langmuir-Blodgett Assembled Graphene Films via Chemical Doping"*	**14:45–15:05**
14:45–15:15	**Bojana Višić** (Serbia), *"Inorganic Nanotubes and Nanowires in Polymer Matrices: Potential for Sensing Applications"*		**Nataša Tomić** (Serbia) *"The Morphological And Structural Changes Of V_2O_5 Cathode Film Upon Electrochemical Cycling"*	**15:05–15:25**
15:15–15:45	**Branislav Nikolić** (USA) *"How ultrafast demagnetization drives spin and charge currents and the ensuing THz radiation"*		**Bojan Stojadinović** (Serbia) *"Role of terbium dopant and oxygen vacancies on conductive properties of $BiFeO_3$ thin films"*	**15:25–15:45**
15:45–16:05		**Coffee Break**		**15:45–16:05**
Chair	**Andrijana Šolajić**		**Igor Pašti**	**Chair**
16:05–16:35	**Mazhar Ali** (Netherlands) *"The Josephson Diode Effect with 2D Kagome Mott Insulators Nb_3X_8 (X = Cl, Br, I)" (online)*		**Marko Spasenović** (Serbia) *"Laser-Induced Graphene on Polymer Substrates for Monitoring Physiological Parameters"*	**16:05–16:35**
16:35–17:05	**Nicola Poccia** (Italy and Germany) *"Exploring quantum complexity in artificially twisted superconducting heterostructures" (online)*		**Enrico Di Lucente** (Switzerland) *"Phonon Boltzmann transport equation beyond the semiclassical regime"*	**16:35–17:05**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 20	Session B – Hall 1	Time
17:05-18:05		**Posters + Cocktail** **SASA Club**		**17:05-18:05**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 21	Session B – Hall 1	Time
Chair	**Bojana Višić**		**Vladimir Dobrosavljević**	**Chair**
09:00–09:30	**Reshef Tenne** (Israel) "Inorganic nanotubes: From WS_2 to 'misfit' compounds"		**Gheorghe-Lucian Pascut** (Romania) *"Crystal Structure Predictions in Correlated Materials at Finite Temperatures"*	**09:00–09:30**
09:30–10:00	**Christoph Gadermair** (Italy) *"Modulation of Ultrafast Quasiparticle Dynamics in Two-dimensional Semiconductors"*		**Louissa Reissig** (Germany) *"The use of differential photocurrent in the characterization of novel optically active materials"*	**09:30–10:00**
10:00–10:30	**Zdenek Sofer** (Czech Republic) *"Novel 2D magnets and dielectrics"*		**Ivna Kavre Piltaver** (Croatia) *"Ultra-thin ZnO coatings on microstructured γ-Fe_2O_3 thin films prepared by atomic layer deposition for enhanced photocatalysis"*	**10:00–10:30**
10:30–10:50	**Coffee Break**			**10:30–10:50**
Chair	**Zdenek Sofer**		**Gheorghe-Lucian Pascut**	**Chair**
10:50–11:20	**Andrew Goodwin**, (UK) *"Truchet-tile architectures in materials design"*		**John Evans** (UK) *"Condensed Matter Physics for Hydrogen Production – the Reversible Memory Reactor"*	**10:50–11:20**
			Sanja Djurdjić Mijin (Spain and Serbia) *"Affordable and Precise Method for Creating Single-Photon Emitters in GaSe"*	**11:20–11:40**
11:20–11:50	**Lena Yadgarov** (Israel) *"Optimized Growth and Manipulation of Light-Matter Interaction in Stabilized Halide Perovskite Nanowire Array"*		**Sonja Predin** (Serbia) *"Pairing Instabilities and Critical States in Graphene Quantum Hall Systems" (Contributed talk)*	**11:40-12:00**
11:50–12:20	**Marija Drndić** (USA) *"Controlling Magnetic Textures in Iron Germanium Telluride (Fe_3GeTe_2) Characterized by Low Temperature Lorentz TEM"*		**Mario Novak** (Croatia) *"Unconventional temperature evolution of quantum oscillations in Sn-doped $BiSbTe_2S$ topological insulator" (Contributed talk)*	**12:00–12:20**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 21	Session B – Hall 1	Time
12:20–14:15	**Lunch Break**			**12:20–14:15**
Chair	**Andres Cantarero**		**Marija Drndić**	**Chair**
14:15–14:45	**Simon Billinge** (USA) *"Tracking local order and dynamics in functional materials"*		**Tomaz Mertelj** (Slovenia) *"Strongly Anisotropic Spinterface Magnetism in Cobalt/Molecular Heterostructures"*	**14:15–14:45**
14:45–15:15	**Jelena Pešić** (Serbia) *"Modeling and Mapping Current Flow in MoS_2 Nanonetworks"*		**Josip Jakovac** (Croatia) *"Electron-plasmon Scattering in Doped Graphene" (Contributed talk)*	**14:45–15:05**
15:15–15:45	**Lev Vidmar** (Slovenia) *"Quantum Phase Transitions Above Ground States: Ergodicity Breaking Transitions"*		**Nikola Stojanović** (Germany) *"Coherent Phonon Raman Spectroscopy as an Emerging Technique for Space Exploration" (Contributed talk)* **Marko Radovic** (Serbia) *"Tunable Electronic States: Semiconductor-to-Metallic state Transition in CeO_2 Nanocrystals"*	**15:05–15:25** **15:25–15:45**
15:45–16:05	**Coffee Break**			**15:45–16:05**
Chairs	**Rudi Hackl, Nenad Lazarević, Slobodan Bubnjević**			**Chairs**
16:05–17:05	**Colloquium** **Peter Hirschfeld** (USA) ***"Superconductivity: there's plenty of cream at the bottom"***			**16:05–17:05**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Time	Session A – Main Hall	May 21	Session B – Hall 1	Time
19:00		**Conference dinner**		**19:00**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 22	Session B – Hall 1	Time
Chair	**Rudi Hackl**		**Myrsini Kaitatzi (WS1)**	**Chair**
09:00–09:30	**Neven Barisic** (Austria and Croatia) *"High-Tc Cuprates – Story of Two Electronic Subsystems"*		**Ana Milosavljević** (Serbia) *"Anisotropic Strain Response in FeSe"*	**09:00–09:30**
09:30–10:00	**Alexandros Lappas** (Greece) *"Fluctuating Magnetic Moments Near Superconductivity in Interlayer-Expanded FeSe"*		**Igor Vaskivskyi** (Slovenia) *"Electron and Lattice Dynamics During Transition to a Metastable Hidden State"*	**09:30–10:00**
10:00–10:30	**László Forró** (USA) *"Aging of High-Tc Superconductors with Defects"*		**Corinna Burri** (Switzerland) *"Imaging of electrically controlled van der Waals layer stacking in 1T-TaS_2"*	**10:00–10:30**
10:30–10:50	**Coffee Break**			**10:30–10:50**
Chair	**Neven Barišić**		**Igor Vaskivskyi (WS1)**	**Chair**
10:50–11:20	**Peter Hirschfeld** (USA) *"Homes scaling across the cuprate phase diagram"*		**Tobias Ritschel** (Germany) *"Charge density waves and superconductivity in Vanadium based Kagome metals" (online)*	**10:50–11:20**
11:20–11:50	**Darko Tanasković** (Serbia) *"Precursors to Anderson Localization in the Holstein Model: Quantum and Quantum-Classical Solutions"*		**Ge He** (China) *"Evidence of spin density wave gap in $La_3Ni_2O_7$"*	**11:20-11:50**
11:50–12:20	**Jonas Bekaert** (Belgium) *"Transition metal dichalcogenides as unique platform for emerging quantum phases: A first-principles perspective"*		**Myrsini Kaitatzi** (Greece) *"Electronically-Driven Local Lattice Distortions in Molecule-Intercalated Iron-Chalcogenide Superconductors"*	**11:50–12:20**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 22	Session B – Hall 1	Time
12:20–14:15		**Lunch Break**		**12:20–14:15**
Chair	**Simon Billinge**		**Tobias Ritschel**	**Chair**
14:15–14:45	**Ivana Radosavljevic Evans** (UK) *"Structure-Property Relationships in Oxide Ion Conductors for Energy Applications"*		**Jure Demšar** (Germany) *"Resilience of Mott Insulating State of La_2CuO_4 Against Photodoping" (online)*	**14:15–14:45**
			Zorica Popović (Serbia) *"Anisotropic Superconductor In Josephson Junction With Rashba Spin Orbit Coupling And Exchange Field"*	**14:45–15:05**
14:45–15:15	**Natalia Drichko** (USA) *"Magnetism and bands topology in $Nd_2Ir_2O_7$ probed by Raman scattering spectroscopy"*		**Valentin Ivanovski** (Serbia) *"Intercalated $ZrTe_3$ by Fe: A Mossbauer Effect Study"*	**15:05–15:25**
15:15–15:45	**Aleksandar Matkovic** (Austria) *"Junctions and Contacts in 2D Semiconductor Devices"*		**Jelena Mitric** (Serbia) *"Invisible Detection with Luminescent Polish for Anti – Counterfeiting"*	**15:25–15:45**
15:45–16:05		**Coffee Break**		**15:45–16:05**
Chair	**Jonas Bekaert**		**Valentin Ivanovski**	**Chair**
16:05–16:35	**Laura Fanfarillo** (Italy) *"Superconductivity in the Presence of Repulsive Interactions"*		**Petar Mitric** (Serbia) *"A Simple and Practical Approach for Calculating Transport Properties with Dynamical Quantum Typicality: Application to the Holstein Model"*	**16:05–16:35**
16:35–17:05	**Birender Singh** (USA) *"Uncovering the Hidden Ferroaxial Orbital Density Wave as the Origin of the Axial Higgs Mode in RTe_3" (online)*		**Zeljko Skoko** (Croatia) *"Harnessing Heat: The Dynamic World of Thermosalient Materials"*	**16:35–17:05**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 22	Session B – Hall 1	Time
17:05-18:05		**Posters + Cocktail** **SASA Club**		**17:05-18:05**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 23	Session B – Hall 1	Time
Chair	**Igor Herbut**		**Emil Božin (WS5)**	**Chair**
09:00–09:30	**Wei Ku** (China) *"Universal low-temperature fluctuation of unconventional superconductors revealed"*		**Cormac McGuinness** (Ireland) *"Neutrons and Photons Elevating Worldwide Science (NEPHEWS) – Trans-National Access For Excellent Curiosity Driven Research"*	**09:00–09:30**
09:30–10:00	**Dragana Popovic** (USA) "*Failed Superconductivity in Chemically Substituted Mott Spin Liquid Materials"*		**Ivana Radosavljevic Evans** (UK) "*Writing Successful Proposals for Beamtime at Large Facilities: Before, During and After the Experiment"*	**09:30–10:00**
10:00–10:30	**Jakša Vučičević** (Serbia) *"Towards numerically exact computation of conductivity in the thermodynamic limit of interacting lattice models"*		**Mads Ry Vogel Jørgensen** (Sweden) *"Material Science using MAX IV – the First 4th Generation Synchrotron Source"*	**10:00–10:30**
10:30–10:50	**Coffee Break**			**10:30–10:50**
Chair	**Darko Tanasković**		**Ivana Radosavljevic Evans (WS5)**	**Chair**
10:50–11:20	**Vladimir Dobrosavljevic** (USA) *"Role of Disorder in Wigner-Mott Transitions"*		**John Evans** (UK) *„Insight on Functional Materials from Parametric Scattering Studies at Large Scale User Facilities"*	**10:50–11:20**
11:20–11:50	**Khandker Quader** (USA) *"Doped Infinite-layer Nickelate Superconductors and Tri-layer Nickelates: Self-consistent DFT+DMFT Approach"*		**Matthias J. Gutmann** (UK) *"Opportunities at the ISIS spallation neutron source"*	**11:20-11:50**
11:50–12:20	**Igor Herbut** *(Canada)* *"SO(8) unified theory of two-dimensional interacting Dirac fermions"*		**Milan Radovic** (Switzerland) *"Spectroscopy at the Synchrotron, Microscopy of the Quantum World"*	**11:50–12:20**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Advances in Solid State Physics and New Materials - May 19–23

Time	Session A – Main Hall	May 23	Session B – Hall 1	Time
12:20–14:15		**Lunch Break**		**12:20–14:15**
Chair	**Alberto Pomar**		**John Evans (WS5)**	**Chair**
14:15–14:45	**Bozidar Nikolić** (Serbia) *"Kagome Thin Layers: Diperiodical Point of View"*		**Michael Gensch** (Germany) *„(Quantum) Materials in high Terahertz Fields"*	**14:15–14:45**
14:45–15:15	**Zorica Konstantinovic** *(Serbia)* *"Nanostructured thin films with strong spin-orbit interaction"*		**Andrew Jackson** (Sweden) *"Future Research Opportunities at European Spallation Source"*	**14:45–15:15**
15:15–15:45	**Snezana Lazić** (Spain) *"Can sound be used for time-bin encoding of photonic qubits for secure quantum communication?"*		**Zurab Guguchia** (Switzerland) *"Muon Spin Rotation: Principles of the Technique and Applications in Quantum Materials Research"* (online)	**15:15–15:45**
15:45–16:05		**Coffee Break**		**15:45–16:05**
Chair	**Bozidar Nikolić**		**Dušan Božanić (WS5)**	**Chair**
16:05–16:35	**Alberto Pomar** (Spain) *"Spin Conduction in FM/AFM/NM Multilayers"*		**Gustavo A. Garcia** (France) *"Photoelectron Circular Dichroism: From Model Molecular Systems to Nanoparticles"*	**16:05–16:35**
16:35–17:05	**Haluk Koralay** (Türkiye) *"Advances in IMD Processed MgB_2 Wires for Potential Applications"*		**Fernando Igoa Saldaña** (Germany) *„High-energy diffraction and scattering for physics and chemistry at PETRA III"*	**16:35–17:05**
17:05–17:35	**Closing ceremony**		**Cormac McGuinness** (Ireland) *"Observing On-Surface Synthesis of Novel Nanostructures By High Resolution Synchrotron Based X-ray Spectroscopies: Chiral Graphene Nanoribbons and Porphyrin Networks"*	**17:05–17:35**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Time	Workshop 2: Advanced Materials in Cultural Heritage Protection, May 22, Hall 2	Time
08:55–09:00	**Workshop opening**	**08:55–09:00**
Chair	**Radmila Panajotović**	**Chair**
09:00–09:20	**Bojana Savić** (Serbia) *"Art Restoration and Science: A Brief History of Entanglement"*	**09:00–09:20**
09:20–09:40	**Aleksa Jelikić** (Serbia) *"Application of Scientific Methodes in Research on Mural Paintings"*	**09:20–09:40**
09:40–10:05	**Bojan Miljević** (Serbia) *"Salt Reduction and Self-Cleaning Protection of Cultural Heritage Objects by Development of New Functional Materials"*	**09:40–10:05**
10:05–10:30	**Nikola Unković** (Serbia) *"Microbial Assisted Biocontrol and Biocleaning in Stone Heritage Conservation - The Case of Rožanec Mithraeum Monument (Slovenia)"*	**10:05–10:30**
10:30–10:50	**Coffee Break**	**10:30–10:50**
Chair	**Jelena Pešić**	
10:50–11:20	**Costas Galiotis** (Greece) *"Science meets Art: graphene enabling solutions for the conservation of cultural heritage"*	**10:50–11:20**
11:20–11:45	**Tijana Tomašević-Ilić** (Serbia) *"Tiled Network Films from Liquid Phase Exfoliated h-BN and Phyllosilicates: Properties and Perspectives for Heritage Protection"*	**11:20–11:45**
11:45–12:10	**Christian Teichert** (Austria) *"Application of Atomic Force Microscopy Based Techniques for Damage Assessment, Conservation, and Restoration of Historical Papers and Fresco Wall Paintings"*	**11:45–12:10**
12:10–14:20	**Lunch Break**	**12:10–14:20**
	Location: Faculty of Applied Arts, University of Arts Belgrade, Kralja Petra 4	
Chair	**Irena Živković**	**Chair**
14:20–14:50	**Tatjana Tripković** (Serbia) *"Portable Spectroscopic Instruments in Analyzing Art and Cultural Heritage: Advantages and Shortcomings"*	**14:20–14:50**
14:50–16:30	**Irena Živković, Ivana Milošević, Jasna Vujin, Bojan Miljević, Milica Pankov, Vesna Miljić, Tatjana Tripković** (Serbia) *"Public training - On-site Demonstration of Artefact Characterization Using Portable Instruments"*	**14:50–16:30**
16:30–16:40	**Workshop closing**	**16:30–16:40**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Time	Workshop 3: Bioaerosols and nanoaerosols: interdisciplinary approaches in microbiology, May 19, Hall 2	Time
Chair	**Predrag Kolarž and Irena Aranđelović**	**Chair**
11:20–11:35	**Irena Aranđelović** (Serbia) *"Introductory talk about the IonCleanTech project and about this workshop"*	**11:20–11:35**
11:35–11:55	**Irena Aranđelović** (Serbia) *"Raising importance of the prevention of transmission of airborne biological matter in indoor air – threats posed by bioaerosols"*	**11:35–11:55**
11:55–12:10	**Marko Janković** (Serbia) *"Respiratory infections of viral etiology in immunosuppressed persons"*	**11:55–12:10**
12:10–12:25	**Stefan Mijatović** (Serbia) *"Allergies of the respiratory tract: fungi as the neglected allergens"*	**12:10–12:25**
12:25–14:15	**Lunch Break**	**12:25–14:15**
Chair	**Predrag Kolarž and Irena Aranđelović**	**Chair**
14:15–14:30	**Irena Aranđelović** (Serbia) *"The lung microbiome – pandemic potential in the era of antimicrobial resistance"*	**14:15–14:30**
14:30–14:45	**Andrea Radalj** (Serbia) *"Animal respiratory viruses with the zoonotic potential"*	**14:30–14:45**
14:45–15:05	**Mira Aničić Urošević** (Serbia) *"Biological Samples for Monitoring of Aerosol and Its Associated Pollutants"*	**14:45–15:05**
15:05–15:25	**Anđelija Ilić** (Serbia) *"Characterization of microplastics using spectroscopic and digital image analyses"*	**15:05–15:25**
15:25–15:45	**Predrag Kolarž** (Serbia) *"Experimental methods for investigation of ion–aerosol interaction"*	**15:25–15:45**
15:45–16:00	**Coffee Break**	**15:45–16:00**
Chair	**Predrag Kolarž and Irena Aranđelović**	**Chair**
16:00–16:20	**Jelena Trajković** (Serbia) *"Carbon–fiber and other ionizer types in combating airborne pathogens – a review"*	**16:00–16:20**
16:20–16:40	**Anđelija Ilić** (Serbia) *"Performance enhancement of HVAC filters by unipolar ionization"*	**16:20–16:40**
16:40–17:00	**Predrag Kolarž** (Serbia) *"Removal and inactivation of bacteria and fungi by ionization / Workshop conclusions"*	**16:40–17:00**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Time	Workshop 4: Computational analysis and modeling of biological materials, May 21, Hall 2	Time
Chair	**Anđelija Ilić and Tijana Štajner**	**Chair**
09:00–09:45	**Vladimir Dobričić** (Serbia) *"Synthesis, physico-chemical and biological properties of acridine derivatives"*	**09:00–09:45**
09:45–10:10	**Tijana Štajner** (Serbia) *"Reinvention of the diagnostic algorithm and treatment options for reactivated toxoplasmosis – ToxoReTREAT project"*	**09:45–10:10**
10:10–10:30	**Olivera Lijeskić** (Serbia) *"Monitoring of reactivated toxoplasmosis in allogeneic HSCT recipients"*	**10:10–10:30**
10:30–10:50	**Coffee Break**	**10:30–10:50**
Chair	**Anđelija Ilić and Tijana Štajner**	**Chair**
10:50–11:10	**Jelena Srbljanović** (Serbia) *"Experimental chemotherapy of reactivated toxoplasmosis"*	**10:50–11:10**
11:10–11:30	**Đorđe Zlatković** (Serbia) *"Cell toxicity and anti-T. gondii efficacy of de novo synthetized acridine derivatives"*	**11:10–11:30**
11:30–11:50	**Anđelija Ilić** (Serbia) *"Cyst recognition in microscopic slides: Estimation of Toxoplasma gondii brain cyst size and location"*	**11:30–11:50**
11:50–12:10	**Jelena Trajković** (Serbia) *"Computational image analysis of developmental dynamics and morphological characteristics of tachyzoites"*	**11:50–12:10**

30-minute talks: 25 min presentation + 5 min Q&A | 20-minute talks: 15 min presentation + 5 min Q&A

Wednesday, May 21, 2025

16:05 – 17:05

Main Hall of Serbian Academy of Sciences and Arts

Colloquium:

Peter Hirschfeld

University of Florida, USA

Superconductivity: there's plenty of cream at the bottom

Abstract. In 1961, Brian Pippard gave a speech at IBM called "The Cat and the Cream", in which he declared that the superconductivity field was finished, at least for "young innocents who wish to break new ground": the cream was gone, and the bowl was empty. I show why the subsequent 6 decades proved him so dramatically wrong, how new materials and experimental techniques have continuously driven new theoretical understandings, such that the field has been repeatedly renewed, and is in fact a very good place for young researchers to make a career.

TABLE OF CONTENTS

1. INVITED TALKS

2. CONTRIBUTED TALKS

3. POSTER SESSION

INVITED TALKS

The Josephson Diode Effect with 2D Kagome Mott Insulators Nb_3X_8 (X = Cl, Br, I)

M. Dubbelman[a,b], H. Wu[a,b], Y. Wang[c], M. Roesner[d], M. N. Ali[a,b]

[a]*Delft University of Technology, Quantum Nanoscience Department, 2628CJ, Delft, Netherlands*
[b]*Kavli Institute of Nanoscience Delft, 2628CJ, Delft, Netherlands*
[c]*KU Leuven, Department of Physics and Astronomy, 3001, Leuven, Belgium*
[d]*Radboud University, Theory of Condensed Matter Department, 6500HC, Nijmegen, Netherlands*

Abstract. Josephson Junctions (JJs) are an important scientific and technological device where two superconductors are coupled together by a non-superconducting barrier, resulting in a sandwich-like heterostructure. Its superconducting properties can be modulated by the barrier or by a magnetic field through the barrier. Recently, great progress has been made in incorporating 2D quantum materials into these structures (QMJJs) where their inherent quantum properties can affect the tunneling superconductivity in novel ways. In this presentation we will discuss some of these results with particular focus on the creation of *non-reciprocal superconductivity* (i.e. one directional) without requiring a magnetic field using 2D Kagome Mott-Insulators Nb_3X_8 (X = Cl, Br, I) as the barrier material. This "Josephson Diode Effect", its relation with the Mott behavior, and other future directions of QMJJ research will be discussed.

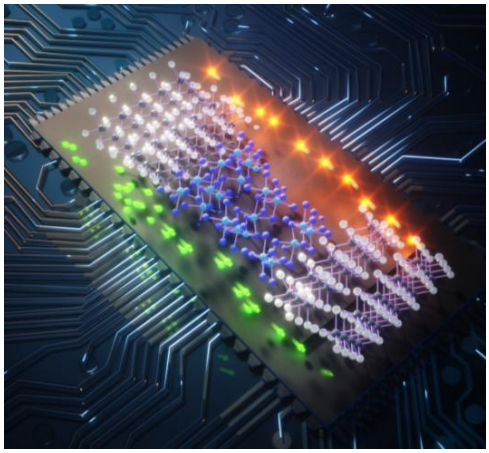

FIGURE 1. Artists rendition of the Josephson Diode Effect in a Quantum Material Josephson Junction. 2 superconductors sandwich a quantum material barrier (crystal structure with blue atoms) and yellow balls depict "slow moving" normal electrons travelling in one direction with green pairs of balls depicting "fast moving" superconducting cooper pairs travelling in the other direction.

Biological Samples for Monitoring of Aerosol and Its Associated Pollutants

Mira Aničić Urošević[a] and Milica Tomašević[a]

[a]*Institute of Physics Belgrade, University of Belgrade, Pregrevica 118, 11080 Belgrade, Serbia*

Abstract. For many years, plants have been studied for their capability to indicate/monitor and remove pollutants from both soil and air [1]. Specifically, vascular tree leaves or mosses can successfully capture aerosol and its associated pollutants. Magnetic biomonitoring using tree leaves has been proven as a proxy for airborne particulate matter (PM) pollution, which has been recognised as an issue of outmost importance for health protection and well-being [2]. Since the leaf entrapment of PM is species-specific, in this study, four tree species common in urban areas of Europe and beyond (*Aesculus hippocastanum*, *Acer platanoides*, *Betula pendula*, and *Tilia cordata*) were investigated to evaluate which biomonitor enables a consistent 'signal' to particle and particle-bound toxic elements. The tree leaves were sampled in the central urban and suburban parks in Belgrade (Serbia) in May and September of four consecutive years. Magnetic PM fractions in the samples were quantified by saturation isothermal remanent magnetization (SIRM), while the concentrations of Al, Cr, Cu, Fe, Ni, Pb, and Zn were determined by inductively coupled plasma optical emission spectrometry (ICP-OES). Magnetic and elemental measurements were considered in comparison to regulatory PM10 data. Median leaf SIRM values of *T. cordata*, *A. hippocastanum*, and *A. platanoides* (174, 140, and $123 \times 10^{-5} \times A\ m^2\ kg^{-1}$, respectively) implied the considerable magnetic enhancement contrary to B. pendula ($68 \times 10^{-5} \times A\ m^2\ kg^{-1}$). However, *B. pendula* leaves showed the significant correlation between SIRM and PM10 values ($r = 0.75$) and SIRM and element concentrations and significant spatio-temporal differences in SIRM/element content between the studied parks/years. These results recommend *B. pendula* as a valuable biomonitor of PM and the associated elements. Nevertheless, both the results (high SIRM values, the significant correlation between SIRM and PM10—$r = 0.71$) and literature findings (abundance, adaptability, PM removal efficiency) favour *A. platanoides* over *B. pendula* in magnetic particle biomonitoring [3].

REFERENCES

1. Markert, B.A., Breure, A.M. and Zechmeister, H.G. (Eds), Bioindicators & Biomonitors, Elsevier Science Ltd. 2003.
2. Grote, R., Samson, R., Alonso, R., Amorim, H.J., Cariñanos, P., Churkina, G., Fares, S., Le Thiec, D., Niinemets, Ü., Norgaard Mikkelsen, T., Paoletti, E., Tiwary, A., and Calfapietra, C., *Front. Ecol. Environ.* **14**, 543–550 (2016).
3. Aničić Urošević, M., Jovanović, G., Stević, N., Deljanin, I., Nikolić, M., Tomašević, M., Samson, R., Leaves of common urban tree species (*Aesculus hippocastanum*, *Acer platanoides*, *Betula pendula* and *Tilia cordata*) as a measure of particle and particle-bound pollution: A four-year study, *Air Qual Atmos Health*, **12** 1081–1090 (2019).

Raising importance of the prevention of transmission of airborne biological matter in indoor air – threats posed by bioaerosols

Irena Arandjelović[a]

[a]*Institute of Microbiology and Immunology, Faculty of Medicine, University of Belgrade*

Abstract. Air pollution in urban environments, as one of the key causes of progressive environmental degradation, is considered a leading ecological threat to human health. Airborne particles composed of biological components forming a stable dispersion system are referred to as bioaerosols. Bioaerosols include viable entities such as fungi, bacteria, and archaea, as well as non-viable entities like viruses, allergens, toxins, and resistance genes. When inhaled, bioaerosols larger than 5 μm tend to deposit in the oral cavity and respiratory tract, increasing the risk of dental caries, gum infections, bronchitis, and bronchiectasis, while those smaller than 5 μm can directly infiltrate the alveoli, leading to the development of various respiratory diseases. As a primary source of atmospheric pathogen transmission, bioaerosols are often associated with the emergence of pandemics and the rapid spread of respiratory infections. Given their nature as complex organic living entities, they are also actively involved in atmospheric processes. It is estimated that current climate changes will lead to an increased incidence of infections caused by threatening respiratory pathogens, primarily because such changes favor airborne transmission, particularly indoors, where people spend up to 90% of their time daily. Moreover, air pollution exacerbates the spatial spread of resistance genes and modulates the temporal patterns of resistance gene expression, which has an undeniable impact on current epidemiological trends in antimicrobial resistance. The complex structure of bioaerosols and their interaction with the human population requires an interdisciplinary approach - integrating knowledge and technologies from epidemiology, microbiology, chemistry, physics, biostatistics, environmental science, and informatics - to effectively prevent bioaerosol transmission.

Acknowledgement. This work has been supported by The Science Fund of the Republic of Serbia, Green program of cooperation between science and industry, grant no. 5661, project acronym – IonCleanTech. Any opinions, findings, conclusions or recommendations expressed are those of the authors and do not necessarily reflect the views of the funder.

REFERENCES

1. Safiri S, Mahmoodpoor A, Kolahi AA, Nejadghaderi SA, Sullman MJM, Mansournia MA, et al. *Front Public Health*. **10**, 1028525 (2023).
2. Salthammer T, Zhao J, Schieweck A, Uhde E, Hussein T, Antretter F, et al. *Indoor Air*. **32**, e13039 (2022).
3. Zhu G, Wang X, Yang T, Su J, Qin Y, Wang S, et al. *ISME J*. **15**, 270-281 (2021).
4. Kolarž P, Ilić AŽ, Janković M, Janićijević A, and Trbovich AM. *J Aerosol Sci*. **173**, 106199 (2023).

The lung microbiome – pandemic potential in the era of antimicrobial resistance

Irena Arandjelović[a]

[a]*Institute of Microbiology and Immunology, Faculty of Medicine, University of Belgrade*

Abstract. Key environmental reservoirs of antimicrobial resistance genes (ARGs) include animal farms, wastewater treatment plants, and hospitals. ARGs are predominantly spread via horizontal gene transfer through mobile genetic elements such as plasmids and transposons. Inhalation represents a relevant exposure route, with adults inhaling up to 10^4 ARG copies daily, mostly via PM2.5 particles, over 80% of which can reach the alveoli. ARGs are emitted into the air through wind, dust, and evaporation, and later redeposited onto surfaces, creating cycles of environmental and human exposure. Air pollution has been linked to increased abundance and diversity of airborne ARGs, as well as to enhanced mobility via gene transfer mechanisms. PM2.5 can promote ARG exchange within the respiratory tract, while ozone exposure may alter airway permeability and microbiota, increasing susceptibility to infections. ARG expression has been detected in 25% of individuals without signs of respiratory infection, indicating a silent potential for resistance development. While not always clinically relevant, persistent environmental exposure may promote phenotypic resistance. These findings position the lung microbiome as a potential reservoir and driver of emerging antimicrobial resistance in the context of urban pollution.

Acknowledgement. This work has been supported by The Science Fund of the Republic of Serbia, Green program of cooperation between science and industry, grant no. 5661, project acronym – IonCleanTech. Any opinions, findings, conclusions or recommendations expressed are those of the authors and do not necessarily reflect the views of the funder.

REFERENCES

1. Chu VT, Tsitsiklis A, Mick E, Ambroggio L, Kalantar KL, Glascock A, et al. *Nat Commun*. **15**, 92 (2024).
2. Li R, Li J, Zhou X. *Signal Transduct Target Ther*. **9**, 19 (2024).
3. Zhu G, Wang X, Yang T, Su J, Qin Y, Wang S, et al. *ISME J*. **15**, 270-281 (2021).

High-T_c Cuprates – Story of Two Electronic Subsystems

Neven Barišić[a,b]

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[b]*Institute of Solid State Physics, TU Wien, Wiedner Hauptstraße 8, 1040 Wien Austria*

Abstract. The experimentally established universalities in high-T_c cuprates will be presented [1-7]. Based on them we show that the phenomenology of cuprates across the phase diagram is fully captured by the simple charge conservation relation:

$$1 + p = n_{loc} + n_{eff}$$

Here, p is the doping while n_{eff} is the carrier density and n_{loc} is the density of localized charge within a CuO_2 plaquette. The corresponding superfluid density is related to both components:

$$\rho_S = n_{eff} \cdot (O_S\, n_{loc}).$$

where all terms can be experimentally determined directly. The charge n_{loc} is responsible for all the strangeness of these compounds, which includes the pseudogap phenomenon and the superconducting glue [8,9].

The compound-dependent constant, O_S, is fine-tuned by the local crystal structure. It arises from the p–d–p fluctuation by the Cu-localized holes visiting the neighboring planar–oxygen atoms and can be determined from NMR [9].

REFERENCES

1. N. Barišić et al., *New J. Phys.* **21**, 113007 (2019); see also arXiv:1507.07885 (2015).
2. Y. Li et a., *Sci. Adv.* **5**, eaap7349 (2019).
3. N. Barišić et al., *Proc. Natl. Acad. Sci. U.S.A.* **110**, 12235 (2013).
4. S. I. Mirzaei et al., *Proc. Natl. Acad. Sci. U.S.A.* **110**, 5774 (2013).
5. M. K. Chan et al., Phys. Rev. Lett. **113**, 177005(2014).
6. P. Popčević et al., *npj Quantum Mater.* **3**, 42 (2018).
7. C. M. N. Kumar et al., *Phys. Rev. B* **107**, 144515 (2023).
8. D. Pelc et al., *Sci. Adv.* **5**, eaau4538 (2019).
9. N. Barišić & D. K. Sunko. *J Supercond. Nov. Magn.* **35**, 1781 (2022).

Transition metal dichalcogenides as unique platform for emerging quantum phases: A first-principles perspective

Jonas Bekaert

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Abstract. Transition metal dichalcogenides (TMDs) are a family of layered van der Waals materials at the forefront of research, owing to their rich polymorphism, diverse electronic properties, facile heterostructuring, and the intricate interplay of emerging quantum phases they exhibit [**? ? ? ?**]. In this talk, we will explore these aspects through first-principles calculations. First, we will show how charge density waves (CDWs) vary drastically depending on the TMD polymorph (T vs. H vs. mixed forms; see Figure 1) [**? ? ?**], and chalcogen composition (S vs. Se) [**?**], comparing first-principles results with Raman spectroscopy [**? ?**] and electron microscopy results [**?**]. Next, we will review the interplay been the CDW state and superconductivity in the 6R-phase of TaS_2, a bulk heterostructure consisting of alternating T and H monolayers. Finally, we will demonstrate that sulfur vacancies in few-layer TMD structures can undergo spontaneous healing through oxygenation, a process that unexpectedly enhances electron-phonon coupling and elevates the superconducting critical temperature [**?**]. This finding highlights a potential pathway for leveraging defect engineering to optimize superconducting properties.

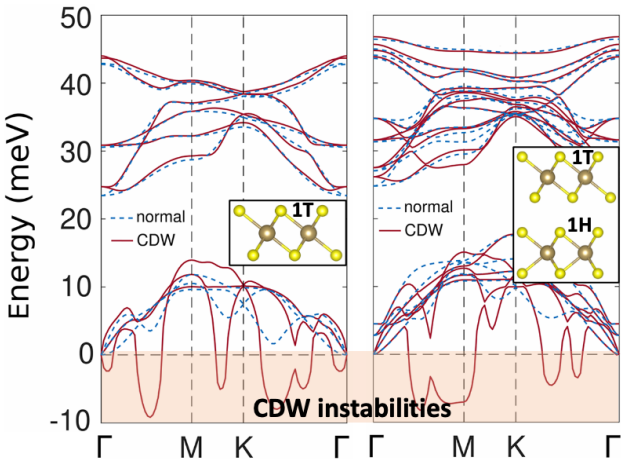

FIGURE 1. Calculated phonon dispersions of (a) monolayer 1T and (b) bilayer 1T-1H of TaS_2, exhibiting charge density wave (CDW) instabilities [**?**]. The orange region indicates imaginary phonon energies, corresponding to evanescent modes that signal a CDW-related lattice reconstruction.

REFERENCES

1. J. Bekaert, E. Khestanova, D. G. Hopkinson, *et al.*, *Enhanced superconductivity in few-layer TaS_2 due to healing by oxygenation*, Nano Letters **20**, 3808 (2020).
2. S. Durdic Mijin, A. Baum, J. Bekaert, *et al.*, *Probing charge density wave phases and the Mott transition in $1T$-TaS_2 by inelastic light scattering*, Physical Review B **103**, 245133 (2021).
3. A. Achari, J. Bekaert, V. Sreepal, *et al.*, *Alternating Superconducting and Charge Density Wave Monolayers within Bulk 6R-TaS_2*, Nano Letters **22**, 6268 (2022).
4. J. Blagojević, S. Djurdjić Mijin, J. Bekaert, *et al.*, *Competition of disorder and electron-phonon coupling in $2H-\mathrm{TaSe}_{2-x}\mathrm{S}_x$ $(0 \leq x \leq 2)$ as evidenced by Raman spectroscopy*, Physical Review Materials **8**, 024004 (2024).

Artificial High Tc Superconductors with Tc amplification on demand made of nano heterostructures by quantum design tuned at a Fano-Feshbach shape resonance

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Abstract. While for 39 years the search of new high Tc superconductors was driven by trial and error methodology here we provide a quantum theory for engineering new cuprate artificial high-Tc superlattices (AHTS) of quantum well thickness L and period d, of few nanometers with Rashba spin-orbit coupling (SOC) tuned at a Fano-Feshbach resonance in multigap superconductors [1,2]. By tuning the geometrical conformational parameter L/d around its magic ratio 2/3 we get the superconducting dome of Tc versus doping controlled by the Fano-Feshbach resonance between two superconducting gaps [3-5]. The sheet resistivity as a function of temperature and high magnetic field shows that the upper critical magnetic field, Hc2, exhibits an upward concavity as a function of temperature, providing compelling evidence of two-band superconductivity and validating the theoretical prediction used in our quantum design. Additionally, we discovered that the L/d ratio influences scattering phenomena in the normal state and by suppressing superconductivity with high magnetic fields, the normal state resistivity shows a low-temperature upturn, providing evidence of the Kondo proximity effect in MIMI superlattices. Finally this novel approach shed finally light on the long standing mysterious mechanism of high temperature superconductivity driven by the Fano-Feshbach quantum shape resonance and the interplay of T-linear resistance competing proximity Kondo scattering in doped Mott insulators. Finally we will discuss the evidence of intrinsic Joseph Junctions in AHTS [6].

REFERENCES

1. Bianconi A., Shape resonances in superstripes. Nature Physics, 9(9), 536-537. (2013).
2. Mazziotti M. V., Bianconi A., Raimondi., R., Campi G., Valletta A.,Spin–orbit coupling controlling the superconducting dome of artificial superlattices of quantum wells, Journal of Applied Physics 132 (2022)
3. Logvenov, G.; Bonmassar, N.; Christiani, G.; Campi, G.; Valletta, A.; Bianconi, A. The superconducting dome in artificial high-Tc superlattices tuned at the Fano–Feshbach resonance by quantum design. Condens. Matter, 8, 78 (2023)
4. Campi, G.; Logvenov, G.;Caprara, S.; Valletta, A.; Bianconi, A. Kondo versus Fano in superconducting artificial high-Tc heterostructures. Condensed Matter 9, 43 (2024)
5. Valletta, A.; Bianconi, A.; Perali, A.; Logvenov, G.; Campi, G. High-Tc superconducting dome in artificial heterostructures made of nanoscale quantum building blocks. Phys. Rev. B 110, 184510 (2024)
6. Ahmad, H. G., Massarottti, D., Tafuri, F., Logvenov, G., Bianconi, A., Campi, G. Josephson coupling in lanthanum-based cuprate superlattices. APL Quantum 2, 016113 (2025) https://doi.org/10.1063/5.0251121

Tracking Local Order and Dynamics in Functional Materials

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Abstract. Total scattering and the atomic pair distribution function (PDF) has been successful at elucidating local structure and atomic short-range order of materials, giving novel insights into real materials including defects and local broken symmetries. However, the PDF does not normally tell you whether disorder that it sees is static or dynamic. Recently we have been thinking of ways to extend total scattering to reveal the time dependence of local structure. I will talk about recent developments for studying local order and dynamics in functional amaterials, including magnetic PDF and a method called variable-shutter PDF where we can use inelastic neutron scattering to systematically change the camera shutter-speed of our PDF measurement, combining inelastic x-ray scattering with PDF to understand structural disorder in hybrid perovskites. Finally, I iwll mention efforts to use machine-learning inspired symmetry adapted filters to extract rotational dynamics of driven skyrmion lattices. All these developments show promise for finding local orders and even giving information on dynamics of the local order to help understand how atoms move in material processes, going beyond knowing just where they are.

Imaging of electrically controlled van der Waals layer stacking in 1*T*-TaS_2

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Abstract.

The layered transition metal dichalcogenide 1*T*-TaS_2 shows many different equilibrium charge density wave (CDW) states upon cooling [1], as well as superconductivity upon application of pressure or doping [2] and even a putative quantum spin liquid state.[3] Furthermore, upon application of sub-picosecond current or femtosecond laser pulses, a metallic 'hidden' CDW state can be induced non-thermally from the insulating commensurate CDW state at low temperatures.[4,5] To directly observe the ultrafast, non-volatile switching of a van der Waals cryomemory cell, we performed three-dimensional (3D), non-destructive imaging of a 1*T*-TaS_2 device at the Swiss Light Source synchrotron.[6] Using a combination of spatially resolved micro-beam X-ray diffraction, fluorescence, and *in-situ* transport measurements, we identify the insulating equilibrium commensurate CDW order, as well as the non-thermal metallic hidden CDW state, induced by electrical switching.

Our results demonstrate that upon excitation a layer restacking occurs and that electrically and optically induced hidden states are structurally and electronically equivalent. Furthermore, 3D tomograms reveal a narrow switching region located beneath and between the electrodes, emphasizing the significance of charge injection and out-of-plane strain in the switching mechanism. These findings provide valuable guidance for optimizing 1*T*-TaS_2 device design and pave the way for non-destructive, bulk-sensitive studies of other phase-change materials using synchrotron light.

REFERENCES

1. J. A. Wilson *et al.*, Adv. Phys. 24, 117 (1975).
2. B. Sipos *et al.*, Nat. Mater 7, 960–965 (2008).
3. M. Klanjsek *et al.*, Nat. Phys. 13, 1130 (2017).
4. L. Stojchevska *et al.*, Science 344, 177 – 180 (2014).
5. I. Vaskivskyi *et al.*, Nat. Commun. 7, 11442 (2016).
6. C. Burri *et al.*, arXiv:2411.04830.

Thickness dependence of the CrI_3 dielectric function

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Abstract. Chromium triiodide (CrI_3) is a magnetic semiconductor with a layered structure where the chromium atoms form a planar arrangement. Each chromium is bonded at the upper and bottom layers to three iodides, the layers being connected by van der Waals forces, giving a quasi-two dimensional character to both the structure and physical properties. In this talk, we will discuss the investigation of the dielectric function of CrI_3 as a function of the number of layers, using hyperspectral imaging techniques. The transmittance data reveals two distinct peaks at approximately 2.7 and 2.0 eV, corresponding to two optical transitions. By analizing the evolution of the imaginary part of the dielectric function, $\varepsilon_2(\omega)$, at these transitions, we identify three different regions: (1) a nanoscale region, where $\varepsilon_2(\omega)$ increases with the number of layers, (2) an intermediate or mesoscopic region, where $\varepsilon_2(\omega)$ undergoes a fast decline, and (3) a bulk-like region, where $\varepsilon_2(\omega)$ saturates. To get deeper insight into these experimental observations, density functional theory (DFT) calculations have been performed, providing both the electronic band structure and the dielectric function.

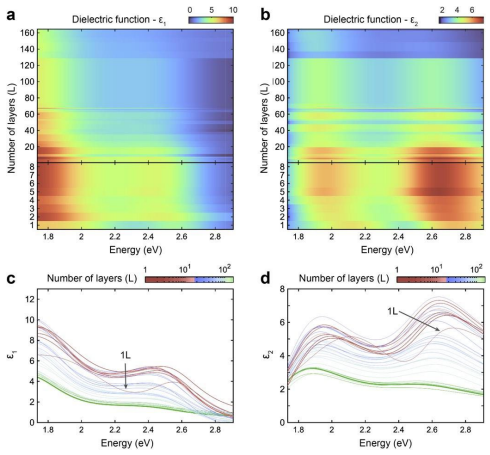

FIGURE 1. Picture to fixed height

REFERENCES

1. Jiang, S. W., Shan, J., and Mak, K. F., *Nature Mater.* **17**, 406 (2018).
2. Djurdjic-Mijin, S. et al, *Phys. Rev. B* **98**, 104307 (2018).
3. Galbiati, M. et al., *Phys. Rev. Lett.* **130**, 146901 (2023).

Group-Theoretical Study of Simple Bands in Two-Dimensional Materials

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Abstract. In two-dimensional materials, simple bands are electronic or phononic bands that do not touch other bands near high-symmetry points of the Brillouin zone. In this contribution we found all possible simple bands in non-magnetic, two-dimensional materials using group theory. We found in total seven types of simple bands including bands of Mexican-hat shape. Our results are shown graphically for cases without and with spin-orbit coupling with the intention to made their usage easier [1].

REFERENCES

1. Damljanović, V., *Existence of Mexican-hat Dispersion and Symmetry Group of a Layer*, Physica E: Low-dimensional Systems and Nanostructures, Vol 170, 116224 (2025).

Optical Signature of Anomalous Hall Effect in a Correlated Magnetic Weyl Semimetal

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Abstract. The interplay of topology with magnetism in Weyl semimetals recently arose to a vanguard topic, because of novel physical scenarios with anomalous transport properties. Here, we address the charge dynamics of the noncentrosymmetric and ferromagnetic (T_C = 15 K) PrAlGe material and discover that it harbours electronic correlations, which get reinforced upon lowering the temperature (T) and induce a renormalisation of the non-trivial bands staging the type I Weyl states [1]. This is reflected in a sizeable reduction of the Fermi velocity with respect to the bare band value. At $T < T_C$, the optical response registers a band reconstruction, which additionally causes a reshuffling of spectral weight (Fig. 1), pertinent to the electronic environment of the Weyl states and scaling with the remarkable anomalous Hall conductivity (AHC). With the support of first-principles calculations, we provide evidence for the intimate relationship between a topological resonance of the absorption spectrum and the progressively enhanced occupation of non-trivial states with large Berry curvatures (Fig. 1), then responsible for AHC in the *dc* limit.

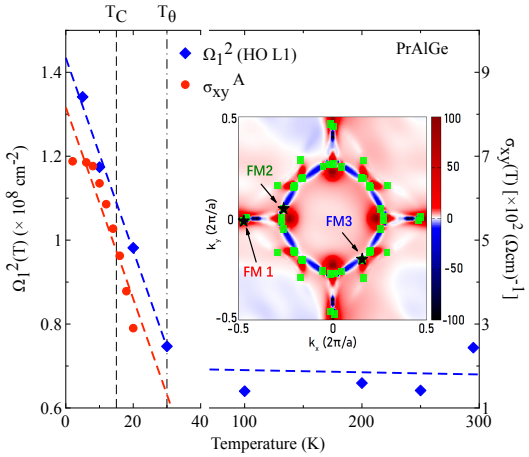

FIGURE 1. Spectral weight (Ω_1^2) versus AHC ($\sigma_{xy} \sim \sigma_{xy}^A$) in PrAlGe. Inset: Effective Berry curvature from our $ab-initio$ calculations, which emphasises its strong enhancement in the ferromagnetic state at those k-points of the Brillouin zone almost coincident with the (projected) Weyl nodes (green symbols).

REFERENCES

1. Yang R., Corasaniti M., Le C.C., Yue C., Hu Z., Hu J.P., Petrovic C., and Degiorgi L., *npj Quantum Materials* **7**, 101 (2022).

Resilience of the Mott Insulating State of La_2CuO_4 against photodoping

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Abstract. The parent compounds of high-T_c cuprate superconductors are Mott insulators with antiferromagnetic (AFM) order, where strong correlations between Cu 3d-electrons split the half-filled Cu 3d-band into the upper (UHB) and lower (LHB) Hubbard band, resulting in an antiferromagnetic insulating ground state [1]. The insulating parent (undoped) compounds are characterized by a charge-transfer (CT) gap of about 2 eV [2] between the oxygen-derived p-band, located within the Mott gap, and the upper Hubbard band (UHB). The nature of doping induced changes in the low energy electronic structure by introducing electrons or holes into the CuO_2 planes is, like the problem of high-Tc cuprates itself, still under intense discussion [1-3]. Introducing a few percent of holes (or electrons) into the CuO_2 planes, results in a transfer of spectral weight to lower energies, with the appearance of excitations in the mid-infrared (MIR) range [2] which eventually merges into the Drude-like free carrier peak near optimal doping [2]. While numerous models have been put forward to account for the doping evolution of free carrier and MIR response, the consensus is still lacking [4]. Photodoping, i.e., generating electron- and hole-like carriers by absorption of light with frequency exceeding the CT gap, was shown to induce similar changes in low energy excitation spectrum to chemical doping, with studies suggesting photoinduced metallic state [5,6]. Here, we investigate transient photodoping in La_2CuO_4, an archetypal antiferromagnetic Mott insulating parent compound of the cuprate high-Tc superconductor by capturing the dynamics of the transient state via tracking the time-evolution of THz photoconductivity and the changes in the complex dielectric function $\varepsilon(\omega,t)$ [7] in the 0.5 – 2.6 eV range in optically-thin films, following optical excitation across the charge transfer (CT) gap. We cover a large range of excitation densities from ~0.001 to ~0.12 absorbed photons [electron-hole pairs] per Cu. Analysis of $\Delta\varepsilon(\omega,t)$ demonstrates a pronounced photoinduced reduction of the CT gap concomitant with the appearance of MIR absorption and a weak free carrier response, all simultaneously relaxing on a (sub)picosecond scale. Up to the highest excitation densities, where at comparable chemical-doping levels a metallic state is realized, the free carrier contribution remains negligible, underscoring the robustness of the underlying electronic correlations. We address the implications of these results to our understanding of weakly doped cuprate superconductors.

REFERENCES

1. Lee, P.A., Nagaosa, N., and Wen, X.G., *Reviews of Modern Physics* **78**, 17-85 (2006).
2. Uchida, S., et al., *Physical Review B* **43**, 7942-7954 (1991).
3. Mishchenko, A.S., et al., *Phys. Rev. Lett.* **100**, 166401 (2008).
4. Leggett, A.J., *Proc. Natl. Acad. Sci. USA* **96**, 8365–8372 (1999).
5. Okamoto, H., et al., *Phys. Rev. B* **83**, 125102 (2011).
6. Baldini, E., et al., *Proc. Natl. Acad. Sci. USA* **117**, 6409–6416 (2020).
7. Obergfell, M., and Demsar, J., *Phys. Rev. Lett.* **124**, 037401 (2020).

Intrinsic Thermal Hall Effect in Mott Insulators

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Abstract. In light of recent experimental data indicating a substantial thermal Hall effect in square lattice antiferromagnetic Mott insulators, we investigate whether a simple Mott insulator can sustain a finite thermal Hall effect. We verify that the answer is "no" if one performs calculations within a spin-only low-energy effective spin model with non-interacting magnons. However, by performing determinant quantum Monte Carlo simulations, we show the single-band t-t′-U Hubbard model coupled to an orbital magnetic field does support a finite thermal Hall effect when $t' \neq 0$ and $B \neq 0$ in the Mott insulating phase. We argue that the (carrier agnostic) necessary conditions for observing a finite thermal Hall effect are time-reversal and particle-hole symmetry breaking. By considering magnon-magnon scattering using a semi-classical Boltzmann analysis, we illustrate a physical mechanism by which finite transverse thermal conductivity may arise, consistent with our symmetry argument and numerical results. Our results contradict the conventional wisdom that square and triangular lattices with SU(2) symmetry do not support a finite thermal Hall effect and call for a critical re-examination of thermal Hall effect data in insulating magnets, as the magnon contribution should not be excluded a priori.

Phonon Boltzmann Transport Equation Beyond The Semiclassical Regime

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Abstract. A detailed understanding of phonon-phonon scattering is essential for predicting key properties such as thermal conductivity in crystals. The semiclassical Boltzmann transport equation (BTE) is a well-established tool for this task, but fails in the overdamped regime, regime where the concept of phonon quasiparticles breaks down. Moreover, the BTE traditionally accounts only for energy-pole phonon propagation—represented by a Lorentzian-shaped spectral function—while neglecting key features observed in many real systems, such as disordered alloys and materials near phase transitions, where spectral functions can exhibit significant satellite peaks. Additionally, BTE calculations often suffer from poor convergence with respect to smearing used to numerically evaluate phonon's scattering rates. To overcome these limitations, we derive from the Kadanoff-Baym equation (KBE) an extended BTE-like equation that includes energy non-conserving scattering events and replaces the numerical smearing with a physical Lorentzian collisional broadening. Exploiting the relation between repumping and depumping scattering, we avoid resummation issues and preserve global energy conservation. We establish a hierarchy of ansätze on Green's and spectral functions, exposing and controlling the approximations needed to ensure smooth transitions from the KBE to the BTE. Importantly, we provide the first rigorous derivation of the time-dependent, non-homogeneous BTE for phonons and demonstrate how our framework naturally accounts for transport contributions from spectral function satellites. This approach is particularly relevant for 2D systems, where standard smearing techniques lack clear convergence, and out-of-plane flexural modes lead to overdamped phonon lifetimes and materials displaying non-Lorentzian spectral features. Our work not only broadens the applicability of the BTE framework but also lays the foundation for future extensions incorporating more complex phonon transport phenomena.

Unlocking the Universality of Fano's Effect in Raman Spectroscopy and Its Role in Condensed Matter Physics

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Abstract. Fano effect, characterized by its distinctive asymmetric spectral profile, remains a cornerstone concept in various branches of modern physics. Initially recognized in atomic systems, this phenomenon has since proven essential in understanding the interplay between discrete and continuum states. In the realm of condensed matter physics, the Fano effect has gained particular importance in the study of conducting systems, where Raman spectroscopy has emerged as a powerful noninvasive tool for probing these interactions. Through Raman scattering, the Fano effect provides critical insight into the coupling between electronic and vibrational states, offering a unique window into the dynamics of charge carriers, excitons, and phonons in materials like graphene, topological insulators, and other nanostructured systems. Furthermore, the role of the Fano effect extends beyond condensed matter, impacting fields such as metamaterials, nanoantennas, and even high-energy physics, where similar mechanisms govern complex phenomena. This presentation will focus on uncovering the universal nature of the Fano Raman spectral lineshape including its relevant nodes, geometrical properties, as well as subtly embedded symmetry features, with an emphasis on its applicability across various materials and systems. The ongoing study will also introduce a comprehensive, yet straightforward fitting procedure that allows experimentalists to efficiently extract critical microscopic parameters from their Raman spectra. The method enables a fairly efficient, rather accurate analysis, directly benefiting researchers in both fundamental studies and applied experimental work.

Affordable and Precise Method for Creating Single-Photon Emitters in GaSe

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Abstract. As quantum technology continues to advance, its applications are expanding beyond the lab into industries, the economy, and everyday life. Ongoing research is bringing us closer to unlocking the full potential of these technologies, which could surpass the limits of today's digital systems. At the heart of this progress are single-photon emitters (SPEs), essential building blocks for quantum technologies such as computing, cryptography, communication, and sensing. Developing a stable and scalable single-photon source is not only a challenge but also a key step toward making quantum technologies widely usable in real-world applications. Among various quantum light sources, defects in two-dimensional (2D) van der Waals materials have emerged as a promising platform due to their tunable energy levels, strong excitonic properties, and efficient charge carrier confinement. 2D SPEs offer high brightness, spectral flexibility, and efficient photon extraction while also operating under normal environmental conditions. Researchers have shown that the way charge carriers are confined in these materials can be controlled by modifying the bandgap using strain or electric fields. In this work, we introduce a cost-effective and practical method to precisely create SPEs in GaSe flakes through strain engineering. Our approach is based on utilizing the optically active microparticles with a unique bipyramidal shape. The bipyramidal shape enhances strain-induced effects crucial for single-photon emitter creation, whereas the optical activity of the particles allows precise identification of their position via conventional optical spectroscopy measurements, eliminating the need for SEM or AFM. Using this method, we successfully created localized SPEs in a thin GaSe flake, resulting in exciton-biexciton cascades with elliptically polarized emission. The presence of excitonic complexes in engineered traps within GaSe sheets suggests that this system could generate entangled photon pairs through an XX-X radiative cascade. Notably, the polarization state of the emitted X-XX cascade can also be controlled by applying external strain or an electric field, further highlights the versatility of this technique. Our results match well with previous studies on strain-induced SPEs in GaSe, confirming the reliability of our method. The introduction of this cost-effective and practical platform for quantum emitter generation expands the accessibility of 2D SPEs, fostering advancements in both research and practical applications

in the field. Overall, our study presents an innovative and cost-effective approach for the deterministic creation of site- and size-controlled single-photon emitters in 2D materials using strain engineering. The adoption of this practical and economically viable technique enhances the accessibility of 2D SPEs, supporting advancements in both fundamental research and real-world quantum applications.

Synthesis, Physico-Chemical and Biological Properties of Acridine Derivatives

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Abstract. Acridine, discovered in 1870 and also known as dibenzo[b,e]pyridine, benzo[b]quinoline, 2,3,5,6-dibenzopyridine, and 10-azaanthracene, is a chemical compound classified as an aromatic heterocycle, consisting of two aromatic rings fused with a central pyridine ring [1]. Although introduced in 19th century, acridine derivatives are still of scientific interest. These molecules can be used in many different spheres, including industry and medicine. Acridine derivatives can be obtained by semi-synthesis of acridines with simpler structure (such as 9-chloroacridine or 9-acridinecarboxaldehyde) or by total synthesis, which enables the introduction of various substituents into the acridine ring. The presence of nitrogen atom in position 10 and conjugated double bonds have significant influence on their synthesis, physico-chemical stability and spectral properties. The most common mechanism of action of acridine derivatives is DNA intercalation, which can lead to functional changes, often to the inhibition of transcription and replication and DNA repair processes. Therefore, serious side effects can be accompanied with their application. However, by careful selection of functional groups that are introduced into the acridine ring, these side effects can be diminished and relatively safe therapeutics could be synthesized. So far published acridine derivatives are mostly tested for antitumor, antibacterial, antiparasitic, antiviral and anti-inflammatory activity [2].

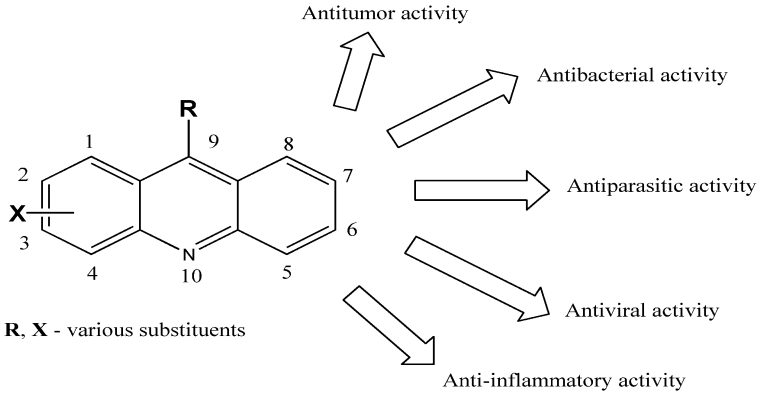

FIGURE 1. Chemical structures and biological activities of acridine derivatives

REFERENCES

1. Marques, D. S. C., da Silva Lima, L., Miranda, J. F. D. O. M., dos Anjos Santos, C. Á., da Cruz Filho, I. J., and de Lima, M. D. C. A. *Bioorg. Chem.* **108096** (2024).
2. Rupar, J., Dobričić, V., Aleksić, M., Brborić, J., and Čudina, O. *Kragujevac J. Sci.* **40**, 83-101 (2018).

Role of Disorder in Wigner-Mott Transitions

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Abstract. Recent work continues to provide mounting evidence of a sharp metal-insulator transition at low electron density, where a Mott-like[1] insulating state forms due to charge ordering (Wigner crystallization). This mechanism has been advocated for a variety of two-dimensional (2D) electronic systems, including electrons at semiconductor interfaces, quasi-2D transition-metal dichalcogenide (TMD) materials such as 1T-TeS_2, but also in a class or recently discovered TMD moire bilayers[2]. In many of these systems, the insulating state seems to be much robust than what is expected for standard Wigner crystallization, bringing into question the corresponding Wigner-Mott physical picture[3]. Here we theoretically explore the role of disorder pinning in stabilizing the Wigner-like charge order, which resolves the key experimental puzzles. We show that disorder pinning suppresses the very soft sheer charge fluctuations, which are generally responsible for the extreme fragility of the Wigner-Mott insulating state.

REFERENCES

1. Y. Tan, V. Dobrosavljevic, L. Rademaker, *How to Recognize the Universal Aspects of Mott Criticality?,* Crystals, **12** (7), 932 (2022).
2. Y. Tan, P. H. Tsang, V. Dobrosavljevic, L. Rademaker, *Doping a Wigner-Mott insulator: Exotic charge orders in transition metal dichalcogenide moire heterobilayers,* Physical Review Research, **5**, 043190 (2023).
3. A. Camjayi, K. Haule, V. Dobrosavljevic, and G. Kotliar, *Coulomb Correlations and the Wigner-Mott Transition,* Nature Physics, **4**, 932 (2008).

Magnetism and bands topology in $Nd_2Ir_2O_7$ probed by Raman scattering spectroscopy.

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Abstract. Pyrochlore iridates present a unique interplay of magnetic frustration, electron correlations, and spin orbit coupling. Weyl semimetal state was suggested in these materials when the quadratic band touching splits into Weyl nodes as a result of time reversal symmetry breaking by the all-in-all-out (AIAO) ordering of the Ir moments. We show that not only $Nd_2Ir_2O_7$ is the best candidate to live up to these theoretical expectations, but due to both A (Nd) and B (Ir) sites of the pyrochlore lattice of this material being magnetic, it demonstrates a unique way to enhance magnetic interactions in the Nd pyrochlore lattice. Using polarized Raman scattering spectroscopy, we can separate the responses of electronic and magnetic degrees of freedom, and follow their temperature dependence down to 7 K through the ordering of Ir moments at T_N^{Ir}= 33 K and of Nd moments below 14 K. A step-like decrease of the electronic scattering at T_N^{Ir} is interpreted as a signature for the splitting of quadratic band touching into Weyl nodes [1]. We detect one- magnon excitations of the AIAO order of Ir moments which appear at T_N^{Ir}. We show that the presence of Ir results in the renormalization of magnetic interactions between Nd moments: Below T_N^{Ir} spin ice fluctuations of Nd magnetic moments are detected through an observation of a collective mode at 15 meV which disappears when Nd moments order in AIAO below 15 K [2]. Phonons evolution through these magnetic ordering transitions evidence for the weak distortion of the lattice at low temperatures.

REFERENCES

1. P. Nikolić et al. Phys. Rev. B **110**, 035148 (2024).
2. Y. Xu et al. arXiv:2302.00579

Controlling Magnetic Textures in Iron Germanium Telluride (Fe_3GeTe_2) Characterized by Low Temperature Lorentz TEM

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Abstract. Iron Germanium Telluride (FGT) is a magnetic van der Waals (vdW) material that has attracted significant interest due to its strong out-of-plane uniaxial magnetic anisotropy and high Curie temperature (T_c ~ 230K) relative to other vdW magnets. These properties make FGT an exciting candidate for spintronics applications. In this study, we probe the effects of geometric confinement on magnetic spin texture in FGT using low-temperature Lorentz transmission electron microscopy (LTEM), a powerful technique which enables direct observation of magnetic domains down to the nanometer scale. Flakes of FGT are mechanically exfoliated from bulk and transferred onto silicon nitride membranes patterned with holes. This results in freestanding regions of FGT, which are subsequently patterned into unique geometries via focused ion beam milling. Samples are initially characterized with a combination of atomic force microscopy, scanning electron microscopy, and optical microscopy. We then perform Lorentz TEM measurements in a JEOL JEM F200 TEM operating at 200 kV. We perform measurements at liquid nitrogen and liquid helium temperatures, using Gatan's Single Tilt Liquid Nitrogen Cryo and Ultra Low Temperature Double Tilt holders, respectively. Our work elucidates the micromagnetic properties of geometrically confined FGT – a key step towards scalable spintronics technology.

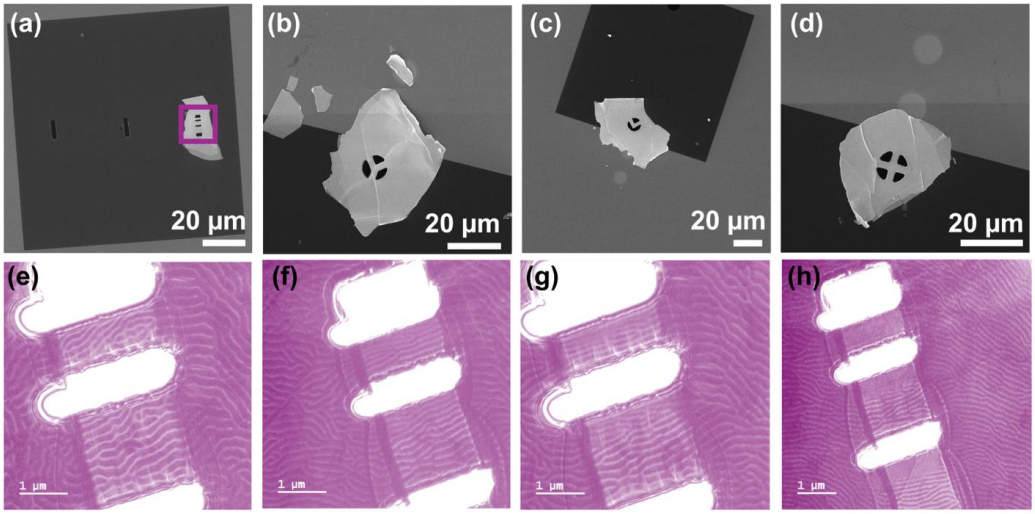

FIGURE 1. Sculpted Fe_3GeTe_2 flakes and corresponding LTEM data. (a-d) Scanning electron microscope images of four devices that have been patterned using focused ion beam milling. (e-h) LTEM temperature series. All images were obtained with a 0.1043T field, 2 mm defocus, and -30° tilt. Panels e, f, g, and h were obtained at 95 K, 133 K, 149 K, and 193 K, respectively.

Condensed Matter Physics for Hydrogen Production – the Reversible Memory Reactor

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Abstract. The water-gas shift reaction (WGS, $CO + H_2O \leftrightharpoons CO_2 + H_2$) is a crucial step in the production of H_2 gas. It is performed on a multimillion-ton scale annually, often as a follow on to steam methane reforming (SMR; $CH_4 + H_2O \leftrightharpoons CO + 3H_2$,) to increase hydrogen yield. The reverse reaction is of equal potential importance in CO_2 capture and its conversion to useful chemical building blocks. The equilibrium constant (K_{eq}) of WGS at the temperature where one might like to work for rapid kinetics and for integration with SMR is $K_{eq} \approx 1.0$ ($T = 820$ C), which means the reaction is inherently inefficient – only 50% of the reactants are converted to products, and significant energy would be needed to separate the mixed gas product stream. In this talk I'll discuss how the defect chemistry of perovskite $ABO_{3-\delta}$ materials in equilibrium with counter flows of the reactive CO and H_2O gases can be used to design a "Memory Reactor". Remarkably, this reactor allows one to "beat" chemical equilibrium limitations and perform the WGS reaction at close-to-100% conversion (super-equilibrium operation). In addition, the design produces naturally separated streams of H_2 and CO_2 product gases, removing the need for subsequent purification. The Memory Reactor is, to our knowledge, the first deliberately-designed reversible reactor and it can instantly switch between WGS and reverse-WGS modes. I'll describe how the reactor operation and its thermodynamic principles can be traced back to phase transitions in the solid-state and concepts such as reversible heat-exchange. I will discuss how we have understood the properties of the reactor and optimized its design using a combination of operando X-ray and neutron (total) scattering studies.

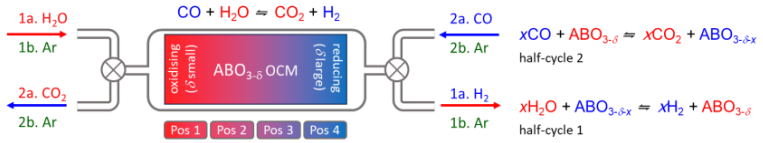

FIGURE 1. A schematic view of the Memory reactor. Pure H_2 gas is produced in half-cycle 1a and pure CO_2 in half-cycle 2a.

REFERENCES

1. Metcalfe, I. S.; Ray, B.; Dejoie, C.; Hu, W.; de Leeuwe, C.; Dueso, C.; García-García, F. R.; Mak, C. M.; Papaioannou, E. I.; Thompson, C. R.; Evans, J.S.O; Overcoming chemical equilibrium limitations using a thermodynamically reversible chemical reactor. *Nature Chemistry* **2019**, *11* (7), 638-643. DOI: 10.1038/s41557-019-0273-2.
2. Telford, D. M.; Martinez Martin, A.; Guy, M. D.; Henry, P. F.; Jones, M. O.; Hu, W.; Metcalfe, I. S.; Evans, J. S. O. Super-equilibrium H_2 production: spatial and time-resolved insight from process and operando neutron diffraction studies of a non-conventional reactor. **2025**, under review.

Insight on Functional Materials from Parametric Scattering Studies at Large Scale User Facilities

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Abstract. X-ray and neutron scattering are amongst the most powerful techniques for understanding the properties of functional materials. The atomic-level insight they provide helps understand how materials function, how they might fail in operation, and ultimately how better materials might be designed. While traditional lab-based experiments often provided a static snapshot of a material under a single set of conditions, experiments at large central facilities such as synchrotrons, neutron sources or XFELs can give invaluable information under non-standard conditions (*in situ* measurements) or as materials function (*operando* measurements). At neutron sources structural studies on the ~30 second timescale might be possible, at synchrotrons on subsecond timescales, while the pulsed nature of XFELs allows processes on the 100 femtosecond level to be followed. In this workshop I'll give examples of how parametric scattering studies under evolving experimental conditions can be performed and the information they provide. Examples will be drawn from work on materials with unusual thermal expansion properties, high ionic conductivity, and important catalytic behaviour. Where possible I'll emphasise how "unusual" or counterintuitive information can be extracted from such studies.

Superconductivity in the Presence of Repulsive Interactions

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Abstract. Multiband superconductors can naturally host repulsive pairing channels, a feature that significantly influences superconducting fluctuations above and below the critical temperature and has a strong impact on experimentally observable quantities. In my talk, I will first outline how repulsive interactions emerge in multiband systems and review established results on their effect on fluctuation behavior. I will then focus on the analysis of the free-energy within the mean-field framework. Recent discussions have raised concerns that the standard mean-field free energy may become unbounded when repulsive channels are present, implying that operative procedures might be required to address this issue. However, by deriving the free-energy variationally, I demonstrate that it remains bounded from below, thereby ensuring the stability of the superconducting solution without the need for any artificial constraints on the order-parameter space. This approach provides a coherent and robust description of the superconducting state in systems where competing interactions are present, and it complements earlier discussions on the subject by offering a clear resolution to the issues arising from standard mean-field treatments.

Aging of High-Tc Superconductors with Defects

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University of Notre Dame

Abstract. Defects, whether magnetic or nonmagnetic, significantly impact superconductivity, sometimes in a detrimental manner. In the high-temperature superconductor $Bi_2Sr_2CaCu_2O_8$ (BiSCO), point defects were introduced via 2.5 MeV fast electron irradiation, with the highest defect concentration estimated to correspond to 1% of Cu displacements. The induced resistivity followed Matthiessen's rule, and the superconducting transition temperature (Tc) exhibited a pronounced decrease. The resistivity evolution was tracked over an unprecedented 20-year timescale. While the superconducting transition temperature remained unchanged, the resistivity steadily increased over time and even exhibited a change in slope. We interpret this behavior as an increase in the effective scattering cross-section of defects over time due to their local chemical reactivity, leading to enhanced backscattering, in alignment with the Mooij correlation. Importantly, we believe this phenomenon is not unique to BiSCO but is likely to extend to other cuprate-based superconductors. These findings raise a critical question: Could other types of defects—such as microstructural breaks formed during the lamination of Ag/BiSCO tapes—also undergo long-term local chemical changes that degrade the performance of superconducting magnets used in various applications?

Acknowledgments: This study is the result of a long-term collaboration involving E. Martino, B. Náfrádi, H. Berger, D. Pavuna, N. Barišić, and many other contributors over the past two decades.

Modulation of Ultrafast Quasiparticle Dynamics in Two-dimensional Semiconductors

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Abstract. Two-dimensional transition metal dichalcogenides (TMDs) combine attractive semiconductor properties and mechanical and chemical robustness with exceptionally strong light-matter interaction. As evidence of this, TMD monolayers with sub-nanometer thickness have demonstrated a range of optical phenomena, including photodetection, photovoltaics, saturable absorption, optical gain, photocatalysis, electrooptical modulation, and optical parametric amplification. Their optical spectra are dominated by two main excitonic resonances A and B. The exciton binding energy is several 100 meV in the monolayer, and is sensitive to screening by charge injection or the dielectric environment.

The functional properties of a material are determined by its response to external stimuli, which drive it out of its equilibrium. As far as electronic and photonic functionalities are concerned, the relevant electron and lattice relaxation processes at the origin of such response occur on the femto- to nanosecond timescale.

We show the modulation of the electron relaxation behaviour upon the application of two external control parameters. Uniaxial tensile strain applied to a TMD monolayer changes the exciton mobility and hence their migration towards defects, which act as recombination centres, thus modulating the exciton lifetimes. Gating TMD monolayers in field effect transistor configuration enables control of the charge density in the material and tweaking the subtle interplay between photoinduced trion formation and exciton dissociation.

Wettability of Covellite

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Abstract. Covellite (covelline) is a copper sulfide mineral (CuS). It has many interesting properties and applications including the first naturally occurring superconductivity or applications for lithium batteries cathodes, ammonium gas sensors or solar cells. In the mining engineering the froth flotation of covellite is an important issue. Therefore, the wettability of covellite (hydrophobicity) is a critical feature. In this this study we used ab-initio methods (density functional theory and molecular dynamics) to calculate the contact angle of covellite (the angle between a liquid and a solid surfaces). It turned out that the calculated value of the contact angle is in a good agreement with the experimental one we measured, proving that ab-initio methods are useful tools in the mining engineering.

Acknowledgement The authors would like to thank Professor Milena Kostovic from Faculty of Mining and Engineering in Belgrade for useful discussions.

REFERENCES

1. P. G. De Gennes, F. Brochard-Wayart, D. Quere, *Capillarity and Wetting Phenomena*, Springer (2004).
2. A. Gross, *Theoretical Surface Science*, Springer (2009).
3. S. R. Rao, J. Leja, *Surface Chemistry of Froth Flotation, 2nd, Vol. 1*, Springer (2004).
4. S. J. Clark, M. D. Segall, C. J. Pickard, P. Hasnip, M. J. Probert, K. Rafson, and M. C. Payne, *Z. Crystallogr*. **220**, 567-570 (2005).
5. A. M. Garcia, J. He, A. L. Soares Jr, and H. A. Duarte, *CrystEngComm*, **19**, 3078-3084 (2017)

Science meets Art: graphene enabling solutions for the conservation of cultural heritage

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[2]*Foundation of Research and Technology – Institute of Chemical Engineering Sciences, Patras, Greece*

Abstract. Tangible cultural heritage is highly vulnerable to degradation. For example, the exposure of paintings to ultraviolet (UV) and visible light, combined with oxidizing agents and other harmful substances, often leads to colour changes such as yellowing or fading. This deterioration is further exacerbated by unfavourable and unstable environmental conditions, harmful lighting, and the presence of pollutants within museum and gallery environments. As a result, scientists are calling for innovative solutions to minimize the risk of damage to cultural heritage artifacts, which represent invaluable legacies of humanity. Over the past few years, our group has been at the forefront of designing and developing graphene-based solutions for the remedial and preventive conservation of tangible cultural heritage. Notably, we have successfully deposited continuous CVD graphene veils onto real paintings without altering their visual appearance, achieving up to a 70% reduction in colour fading [1]. Additionally, by utilizing graphene and related materials in powder form (e.g., GNP, GO), we have developed paints for applications in art and architecture. These paints not only possess intrinsic anti-fading properties but also offer multifunctional benefits [2]. Furthermore, we have created intelligent solutions to monitor and regulate environmental conditions for storing and displaying artworks. These include graphene-based sensors for the early detection of humidity and temperature fluctuations, as well as aggressive species such as volatile organic compounds (VOCs) [3,4]. We have also developed graphene aerogels with exceptional VOC absorption capabilities and antifungal activity, providing effective protection against common threats like fungi and other pollutants [5,6].

REFERENCES

1. Kotsidi et al. Nature Nanotechnology 16, 1004 (2021)
2. Kotsidi et al., Nanoscale 15, 5414 (2023)
3. Paterakis et al., Nanomaterials 12, 2684 (2022)
4. Matsalis et al., Sensors International 5, 100272 (2024)
5. Gorgolis et al., ChemNanoMat 8, e202200265 (2022)
6. Gorgolis et al., Materials 17, 3174 (2024)

Ultrafast Raman Scattering in Quantum Materials

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Abstract. Controlling materials properties with light pulses is an emerging field in condensed matter research. Quantum materials with their delicate interplay of magnetic, electronic, orbital and lattice degrees of freedom offer an attractive playground to demonstrate optically induced novel phases out-of-equilibrium with unique properties.

To achieve this, spectroscopic techniques capable of probing electronic, magnetic and lattice degrees of freedom on the ultrafast timescales (picosecond or femtosecond), both table-top and in large scale facilities, are currently being developed. In this talk, I will discuss the extension of Raman scattering to the ultrafast time scale as a symmetry resolved probe of non-equilibrium lattice and electronic properties of quantum materials[1]. Quite remarkably this well-established technique to probe quantum materials in equilibrium has remained relatively underused on the ultrafast time scale. After a brief introduction to the technique, I will illustrate its use the study the out-of-equilibrium dynamics of the excitonic insulator candidate Ta_2NiSe_5, superconducting cuprates and transition metal di-chalcogenide displaying charge density wave order[2].

REFERENCES

1. K. Katsumi et al. Phys. Rev. Lett. 130, 106904 (2023)
2. L. Gatuingt et al., in preparation (2025)

Photoelectron Circular Dichroism: From Model Molecular Systems to Nanoparticles

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Abstract. Since the first experimental and theoretical demonstration at the turn of the century, photoelectron circular dichroism (PECD)—a photoemission asymmetry along light's propagation axis occurring within the electric dipole approximation [1]—has become the technique of choice to study chirality in the gas phase, both in the frequency and time domains, due to the large dichroic signals of up to 40%. I will trace the developments of the field, mainly focusing on valence-shell photoionization, by first describing its properties as inferred from small, rigid model molecules such as the one pictured in Figure 1 before discussing more increasingly complex systems like radicals, clusters, or nanoparticles. If time allows, analytical perspectives will also be examined.

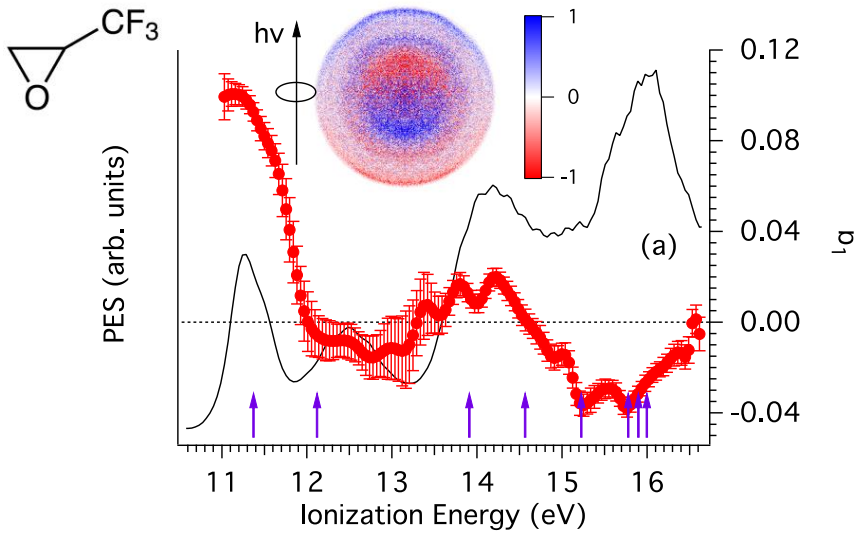

FIGURE 1. PECD (= $2b_1$, red points) and photoelectron spectrum (black line) curves for the S-trifluoromethyloxirane recorded at a photon energy of 17 eV. The corresponding raw difference photoelectron image is shown as an inset. The synchrotron light propagates from south to north of the image. Violet arrows represent the calculated vertical ionization energies.

REFERENCES

1. L. Nahon, G. A. Garcia, and I. Powis, J. Electron Spectrosc. Relat. Phenom. **204**, 322 (2015)

Elastic lattice tuning and magnetic interactions of Kitaev materials

Jochen Geck

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Abstract. Layered materials continue to offer a fertile ground for discovering emergent phenomena driven by electronic correlations and topology. Among the most intriguing of these are Kitaev quantum spin liquids (QSLs), which host exotic states arising from bond-dependent magnetic interactions on honeycomb lattices.

In this talk, I will discuss our recent work on two candidate Kitaev materials—α-$RuCl_3$ and $Na_3Co_2SbO_6$—which exemplify distinct pathways toward realizing a Kitaev QSL. By combining elastic lattice tuning with advanced X-ray scattering techniques and theoretical modeling, we uncover new insights into the pressure-dependent evolution of the lattice and its role in shaping magnetic frustration. Our results reveal important aspects of interplay between lattice structure and magnetism and suggest that the conventional superexchange framework commonly applied to Kitaev materials needs to be extended in the studied as well as other materials.

(Quantum) Materials in high Terahertz Fields

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Abstract. High Terahertz fields have recently become available from laser-driven table-top sources but also from accelerator-based superradiant Terahertz sources. Electric Fields of up to MV/cm or magnetic fields of few 100 mT are thereby available in ultra-short bursts on femtosecond time scales. In particular the accelerator-based facilities provide these fields also in a spectrally tunable fashion, which allows to address low energy degrees of freedom selectively [1].
In my talk I will introduce a class of compact superradiant linac-based terahertz facilities [2] which are now coming into operation worldwide on the example of the TELBE facility [3] in Germany. I will discuss the enormous scientific potential based on selected work on quantum materials such as Graphene [4,5,6], Topological Insulators [7] and Superconductors [8]. I will also give a forecast of future developments and potential applications in the life sciences.

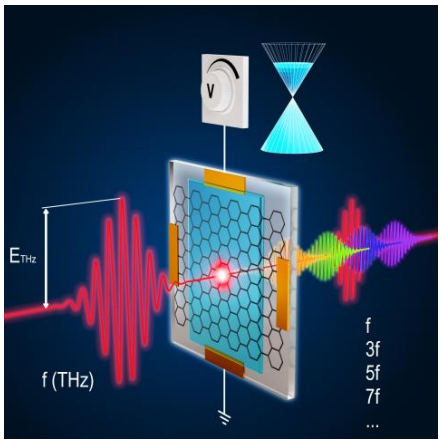

FIGURE 1. Discovery of electrically tunable THz nonlinearity of graphene [6] ©Juniks/HZDR

References

1. S. Kovalev et al., Selective THz control of magnetic order: new opportunities from superradiant undulator sources, *J. Phys. D* **51**, 114007 (2018).
2. M. Gensch, Super-radiant Linac-based THz Sources in 2013, *Proc. of FEL2013*, NY, USA, WEIBNO01.
3. B. Green *et al.*, High-Field High-Repetition-Rate Sources for the Coherent THz Control of Matter. *Sci Rep* **6**, 22256 (2016).
4. H.A. Hafez *et al.* Extremely efficient terahertz high-harmonic generation in graphene by hot Dirac fermions. *Nature* **561**, 507–511 (2018).
5. J.-C. Deinert et al., Grating-Graphene Metamaterial as a Platform for Terahertz Nonlinear Photonics, *ACS Nano* **15**, 1145-1154 **(**2021**).**
6. S. Kovalev *et al.* Electrical tunability of terahertz nonlinearity in graphene. *Sci. Adv.***7**, eabf9809 (2021).
7. S. Kovalev *et al.* Terahertz signatures of ultrafast Dirac fermion relaxation at the surface of topological insulators. *npj Quantum Mater.* **6**, 84 (2021).
8. H. Chu *et al.* Phase-resolved Higgs response in superconducting cuprates. *Nat Commun* **11**, 1793 (2020).

Truchet-tile architectures in materials design

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Abstract. Truchet tilings are periodic arrangements of tiles decorated to lower their symmetry [1]. A generalised version of barcodes and QR codes, they combine elements of order and disorder in a way that allows efficient information storage [2]. This talk will explore the way in which the complex structures of some solid-state compounds – including a heavily disordered metal–organic framework [3] – can be understood in the context of Truchet tilings, and the prospect for exploiting Truchet's approach as a central principle in the design of disordered materials with unconventional electronic, vibrational, and mechanical properties [4,5].

REFERENCES

1. Truchet, S., *Mém. Acad. R. Sci. (Paris)*, 1704, 363-372.
2. Smith, C. S., and Boucher, P. *Leonardo* **20**, 373-385 (1987).
3. Meekel, E. G., Schmidt, E. M., Cameron, L. J., Dharma, A. D., Windsor, H. J., Duyker, S. G., Minelli, A., Pope, T., Orazio Lepore, G., Slater, B., Kepert, C. J., and Goodwin, A. L. *Science* **379**, 357-361 (2023).
4. Roth, N., and Goodwin, A. L., *Nat. Commun.* **14**, 4328 (2023).
5. Meekel, E. G., Partridge, P., Paraoan, R. A. I., Levinsky, J. J. B., Slater, B., Hobday, C. L., and Goodwin, A. L. *Nat. Mater.* **23**, 1245-1251 (2024).

Unconventional Superconductivity and Charge Order in Kagome Lattices Revealed by Muon Spin Rotation

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Abstract. Kagome lattices stand at the forefront of research due to their fascinating interplay of topology, correlations, and magnetism [1-3]. In my talk, I aim to shed light on the latest experimental developments concerning superconductivity and the magnetic aspects of charge order in various kagome-lattice systems, studied from the perspective of local magnetic probe. This involves the use of muon-spin rotation (μSR) as a function of depth from the sample surface and under extreme conditions like hydrostatic pressure, uniaxial strain, ultra-low temperatures, and high magnetic fields. μSR is complemented by magnetoresistance and X-ray diffraction techniques. Key systems under discussion will include: (1) The AV_3Sb_5 (A = K, Rb, Cs) compound series with V kagome lattice, notable for displaying a range of symmetry-breaking electronic orders [4], such as charge order and superconductivity. Here, we have identified a depth-tunable time-reversal symmetry-breaking state associated with charge order [5-9]. Additionally, we have found a chain of evidence for unconventional superconductivity [6-10]. (2) The bilayer kagome material ScV_6Sn_6, where hidden magnetism within the charge-ordered state was observed [11]. (3) The $LaRu_3Si_2$ system with Ru kagome layers, in which we identified two distinct types of charge order (bond order), with one manifesting above room temperature [12,13]. Furthermore, we discovered a dome-shaped superconducting phase diagram under pressure, linked to charge order [14].

REFERENCES

1. I. Syozi, Prog. Theor. Phys. **6**, 306 (1951).
2. S.D. Wilson and B.R. Ortiz, arXiv:2311.05946 (2023).
3. Z. Guguchia et. al., Nature Communications **11**, 559 (2020).
4. T. Neupert et. al., Nature Physics **18**, 137 (2022).
5. C. Mielke III, et. al., and Z. Guguchia, Nature **602**, 245 (2022).
6. Z. Guguchia et. al., Nature Communications **14**, 153 (2023).
7. Z. Guguchia et. al., NPJ Quantum Materials **8**, 41 (2023).
8. J.N. Graham et. al., and Z. Guguchia, Nature Communications 15, 8978 (2024).
9. J.N. Graham et. al., and Z. Guguchia, arXiv:2411.18744 (2024).
10. H. Deng, G.L., Z. Guguchia et. al., and J. Yin, Nature Materials (2024).
11. Z. Guguchia et. al., Nature Communications **14**, 7796 (2023).
12. I. Plokhikh et. al., and Z. Guguchia, Comm. Physics **7**, 182 (2023).
13. C. Mielke III, V. Sazgari, et. al., and Z. Guguchia, arXiv:2402.16219 (2024).
14. K. Ma, et. al., S. Medvedev and Z. Guguchia, arXiv:2412.05459 (2024).

Muon Spin Rotation: Principles of the Technique and Applications in Quantum Materials Research

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Abstract. Muon Spin Rotation (μSR) (see Figure 1) is a powerful probe for investigating magnetic and superconducting properties at the microscopic level [1-4]. The technique exploits the interaction of implanted spin-polarized muons with local magnetic fields, providing direct insights into internal field distributions, electronic correlations, and order parameters in quantum materials. μSR is particularly valuable for studying unconventional superconductors, time-reversal symmetry-breaking charge orders, quantum spin systems, and emergent phases under extreme conditions such as strain, pressure, and low temperatures. This talk outlines the fundamental principles of μSR, its experimental methodologies, and key applications in exploring exotic quantum states in correlated electron systems [1-3].

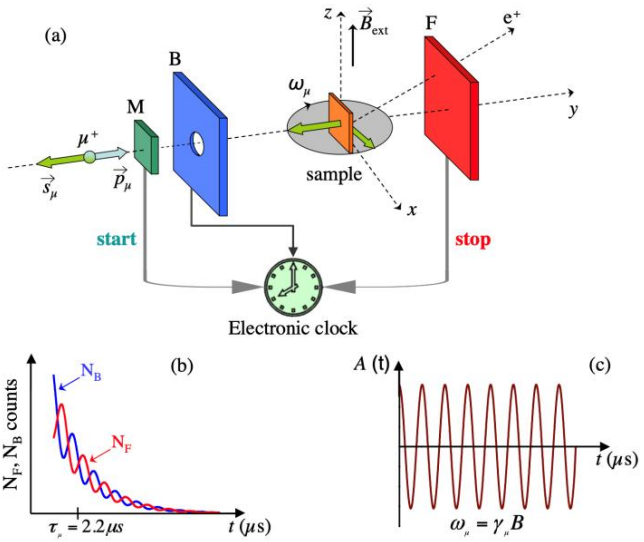

Figure 1: Principle of a μSR experiment. (a) overview of the experimental setup. Spin polarized muons with spin S_μ antiparallel to the momentum p_μ are implanted in the sample placed between the forward (F) and the backward (B) positron detectors. A clock is started at the time the muon enters the muon detector (M) and stopped as soon as the decay positron is detected in detector F or B. (b) The number of detected positrons N_F and N_B as a function of time for the forward and backward detector, respectively. (c) The typical asymmetry signal.

References

1. Z. Guguchia et. al., NPJ Quantum Materials **8**, 41 (2023).
2. C. Mielke III, et. al., and Z. Guguchia, Nature **602**, 245 (2022).

3. Z. Guguchia et. al., Nature Communications **14**, 153 (2023).
4. A. Amato and E. Morenzoni, Introduction to Muon Spin Spectroscopy: Applications to Solid State and Material Sciences (Springer, 2024).

Opportunities At The ISIS Spallation Neutron Source

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Abstract. The ISIS spallation neutron source is a world-leading research center near Oxford welcoming users from all over the world and celebrating its 40th anniversary in 2025. It is part of the Harwell campus at the Rutherford Appleton Laboratory which is hosting several large-scale facilities providing complementary techniques to investigate condensed matter. Techniques include single crystal and powder diffraction, imaging, spectroscopy, small-angle scattering, reflectometry, and deep inelastic neutron scattering supported by computational modelling and a dedicated materials characterization laboratory. In this talk, I will give an overview over the techniques available, showcase some examples and provide tips on how to apply for beamtime.

FIGURE 1. Aerial view of the Rutherford Appleton Laboratory. The ISIS spallation neutron source with its two experimental halls is located at left. The DIAMOND synchrotron is the prominent ring at the right.

Evidence of spin density wave gap in $La_3Ni_2O_7$

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Abstract. Charge and spin density wave orders have garnered significant attention in the study of high-Tc superconductivity, as they are expected to be strongly correlated. In the newly discovered nickel oxide superconductors, density wave order has been observed in various experiments [1–3], though its underlying mechanism remains an open question. Here, we systematically investigate $La_3Ni_2O_7$ at ambient pressure using polarization-dependent inelastic light scattering. We identify several Raman-active phonon modes. The temperature dependence of phonon frequency and linewidth exhibits no anomalies in the range of 50 K to 300 K. In the electronic continuum, however, an unexpected redistribution of spectral weight is observed in both the A_g and B_{1g} symmetries. Specifically, in the A_g channel, a slight loss of spectral weight occurs below 350 cm^{-1} (43.7 meV). In contrast, a gap-like feature is clearly observed in the symmetry, with a peak at approximately 650 cm^{-1} (81.2 meV). The redistribution of spectral weight vanishes around 150 K, with residual intensity peaking at 570 cm^{-1} at higher temperatures and gradually diminishing as the temperature increases. These findings support spin density wave order as the dominant ordering in $La_3Ni_2O_7$, arising from $Q=(\pi/2, \pi/2)$ Fermi surface nesting. This result provides key insights into the superconducting mechanism of nickelates.

REFERENCES

1. Rustem Khasanov, Thomas J. Hicken, Dariusz J. Gawryluk *et al.*, *Nat. Phys.* **21,** 430-436 (2025)
2. Yanghao Meng, Yi Yang, Hualei Sun *et al.*, *Nat. Commun.* **15,** 10408 (2024)
3. Zhe Liu, Mengwu Huo, Jie Li *et al.*, *Nat. Commun.* **15,** 7570 (2024)

SO(8) Unified Theory of Two-Dimensional Interacting Dirac Fermions

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Abstract. Dirac fermions appear as low-energy quasiparticle excitations in many condensed matter systems of current interest. They are often weakly interacting, as in graphene for example, but at intermediate interactions they can also exhibit many ordered ground states by going through phase transitions at which gapless Dirac fermions play a crucial role. A prime example of such a transition occurs in the standard Hubbard model on honeycomb lattice at half filling, which has a semimetal - Mott insulator transition in the so-called Heisenberg-Gross-Neveu universality class. [1] I will discuss a unifying theory of leading order parameters for Dirac systems in two-dimensions, based on the hidden SO(8) symmetry in the Majorana representation of the problem. [2] The phenomena such as doping-induced insulator-superconductor transition, and new critical fixed points induced by Dirac fermions [3] will be discussed time permitting.

REFERENCES

1. I. F. Herbut, Interactions and phase transitions on graphene's honeycomb lattice, Phys. Rev. Lett. **97**, 146401 (2006).
2. I. F. Herbut and S. Mandal, SO(8) unification and the large-N theory of superconductor-insulator transition in two-dimensional Dirac fermions, Phys. Rev. B **108**, L161108 (2023).
3. S. Han and I. F. Herbut, Spontaneous breaking of the SO(2N) symmetry in the Gross-Neveu model, Phys. Rev. D **109**, 096026 (2024); Gross-Neveu-Yukawa theory of SO(2N) to SO(N) X SO(N) spontaneous symmetry breaking, Phys. Rev. B **110**, 125131 (2024).

Optical Transitions Between Entangled Electron-Phonon States

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Abstract. Silicon, a cornerstone material in electronics and photonics, exhibits a diamond crystal structure with two atoms per unit cell and three optical phonons. These phonons, however, remain inaccessible to conventional linear optical techniques. Here we demonstrate that time-resolved pump-probe spectroscopic ellipsometry (TRSE) [1] can overcome these limitations, enabling the detection of optical phonon responses in silicon at both the BZ center and edge. Using pump pulses with photon energies below the indirect bandgap of silicon, we leverage two-photon absorption (TPA) to induce sub-bandgap excitation.

Broadband transient optical effects were probed in the 1.9–3.6 eV spectral range with pump-probe time delays from 50 fs to 4.5 ns. We observed for each pump photon energy (0.95 eV, 1.08 eV, 1.18 eV, 1.27 eV) three distinct features: (i) a broadband spectral structure exhibiting a right-tilted "S" shape at the E_1 critical point, with negative and positive changes at different energy ranges, persisting for up to 4.5 ns; (ii) longitudinal optical (LO) phonon replicas with a characteristic energy spacing of 57 ± 9 meV [3], visible in the 2.9–3.3 eV range and lasting approximately 300 fs; and (iii) two-phonon replicas, exhibiting a spacing of 81 ± 7 meV, observed in the 2.2–2.5 eV range and following a similar temporal evolution as the LO phonon replicas. For approximately 300 fs, coherent oscillations of electrons and nuclei manifest as phonon replicas superimposed on electronic transitions, providing direct evidence of entangled electron-phonon states.

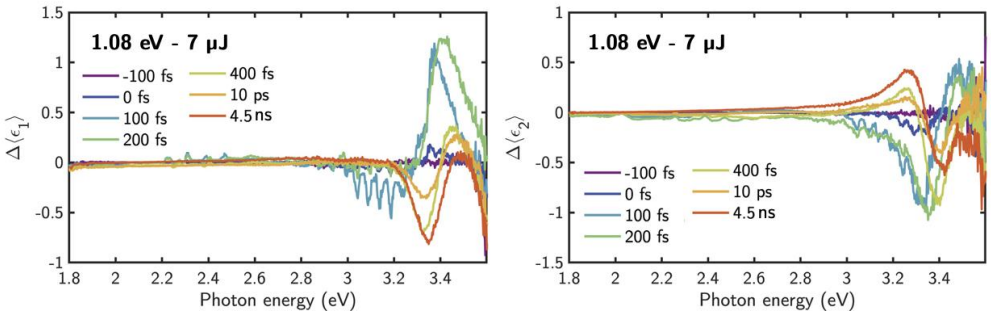

FIGURE 1. Transient real and imaginary part of the pseudo dielectric function $\Delta\langle\epsilon_1\rangle$ and $\Delta\langle\epsilon_2\rangle$ for different time delays. The pump photon energy and pump energy are 1.08 eV and 7 µJ.

REFERENCES

[1] Richter, S. *et al.* New J. Phys. 2020, 22 (8), 083066
[2] M. Spasenović, *et. a.l* Phys. Rev. B77, 085201 (2008)
[3] *Group IV Elements, IV-IV and III-V Compounds. Part b - Electronic, Transport, Optical and Other Properties*; Madelung, O., Rössler, U., Schulz, M., Eds.; Landolt-Börnstein
[4] *Ultrafast Spectroscopy of Semiconductors and Semiconductor Nanostructures*, Jagdeep Shah 2nd ed. Springer (1999)

Homes scaling across the cuprate phase diagram

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University of Florida

Abstract. Beginning with high- T_c cuprate materials, it has been observed that many superconductors exhibit so-called "Homes scaling", in which the zero-temperature superfluid density, ρ_s0, is proportional to the product of the normal-state dc conductivity and the superconducting transition temperature, σ_dc T_c. For conventional, s-wave superconductors, such scaling has been shown to be a natural consequence of elastic-scattering disorder, but we show that when an analogous calculation is carried out for elastic scattering in d-wave superconductors, a stark contrast emerges, with ρ_s0∝(σ_dc T_c)^2 in the dirty limit, in apparent violation of Homes scaling. Within a simple approximate Migdal-Eliashberg treatment of inelastic scattering, I show how Homes scaling is recovered. In addition, I a revised analysis where both axes of the original Homes scaling plot are normalized by the Drude plasma weight, ω_(p,D)^2, and argue that this represents a powerful new tool for classifying superconductors in terms of order parameter symmetry, as well as scattering strength and character.

*work performed with D. Broun, S. Dodge, and V. Mishra

High-energy diffraction and scattering for physics and chemistry at PETRA III

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Abstract. The beamlines P07-DESY & P21.1, located at the PETRA III synchrotron radiation source in Hamburg, Germany, stand as versatile platforms for high-energy X-ray scattering studies. Both beamlines are designed to serve a diverse range of communities by offering advanced techniques for structural insights into powders, thin films and single crystals, including composites and devices. The beamlines operate at X-ray energies between 50 and 120 keV. Such high energies permit the measurement through complex and voluminous sample environments, while still being able to access high momentum transfer (q) ranges. Therefore, the beamlines are particularly active in carrying out in situ scattering experiments. The experimental hutch at P21.1, depicted in Figure 1 as an example, houses a heavy load diffractometer capable of carrying loads up to 600 kg with large dimensions. Available standard sample environments include high temperature furnaces (up to 1500 °C), low temperature cryostats (down to 2 K) and scattering chambers for low background measurements. Moreover, user-provided setups are easily adaptable to the beamlines. Applications examples include in situ nanoparticle growth in wet-chemical synthesis studied through pair-distribution function, local disorder and symmetry breaking characterization by single-crystal diffuse scattering and3D-Δpdf, operando diffraction tomography studies in commercial batteries, complex phase diagrams determined in correlated electron materials through diffraction at low temperature and high magnetic field, among many others. In this talk, the P07-DESY and P21.1 beamline capabilities along with specific scientific examples will be presented to demonstrate the array of techniques available for the user community.

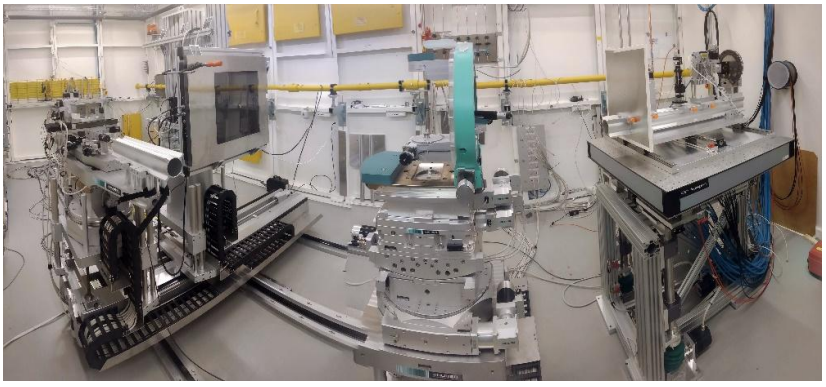

FIGURE 1. P21.1 Control hutch layout. The X-ray beam comes from the right-hand side and shines the sample at the sample tower position at the center. The scattered signal is then detected by the large area 2D detector at the left.

Applications of Small Air Ions and Electromagnetic Fields in Research with Biological Materials

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Abstract. With the shift of focus of biomedical research towards preventive and personalized medicine, properties and interactions of biological materials have attracted increased attention. Part of our research topics deal with structural alterations due to either a disease or an external influence. A large part of topics includes optimization of approaches and exposures, as well as the custom device design, aimed at achieving certain effects of exposures of biological materials to small air ions and/or electromagnetic (EM) fields [1], [2]. Low velocity air ions have short half-life times and exert electrostatic influence. We have studied their interaction with bioaerosols. We have also designed high-frequency EM components and circuits for communications and biomedicine. Some of the resulting effects to biological materials will be described.

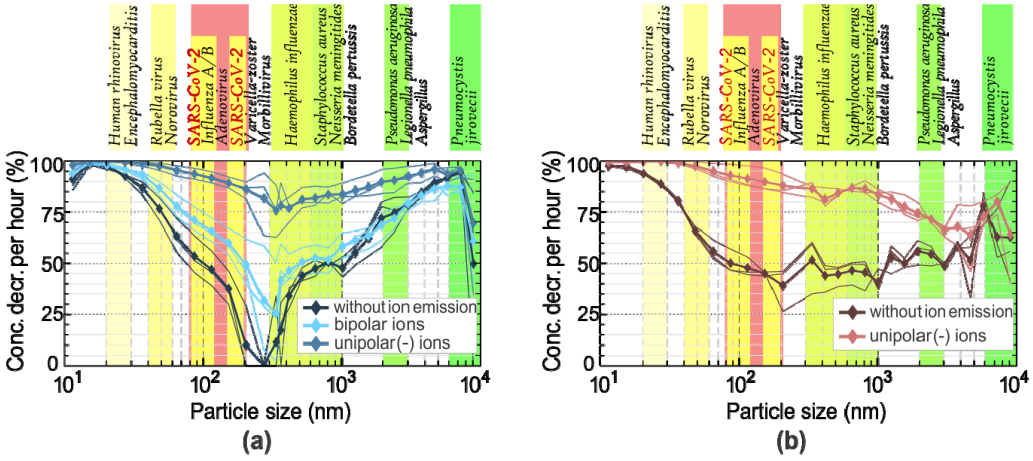

FIGURE 1. Particle number concentration decrease per hour (aerosol deposition without ions, with bipolar ions, with negative air ions): (a) NaCl solution, (b) cigarette smoke. (Please see [1]).

REFERENCES

1. Kolarž, P., Ilić, A.Ž., Janković, M., Janićijević, A., Trbovich, A.M., *J Aerosol Sci*. **173**, 106199 (2023).
2. Ilić, A.Ž., Bukvić, B.M., Stojiljković, M., Skakić, A., Pavlović, S., Jovanović, S.P., Ilić, M.M., *J. Phys. D: Appl. Phys*. **54**, 505401 (2021).

Characterization of Microplastics using Spectroscopic and Digital Image Analyses

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Abstract. Accumulation of plastics in the environment is one of the major environmental problems. Microplastics has been shown to pose risks and hazards both to the human health and to the environment [1]. Aiming to better understand its degradation efficiency, we have investigated the changes in the optical properties of polypropylene (PP), polyethylene (PE), and polystyrene (PS), when exposed to different treatments: ozone, UV radiation, and plasma. The resulting changes have been analyzed using FTIR and Raman spectroscopy [2]. The gained insights could be used to optimize microplastics treatment, or to plan more general degradation protocols. Additionally, the possibility to employ computational image analysis alongside microscopic techniques for microplastics characterization and classification [3] will be discussed.
Acknowledgement. This work has been supported by The Science Fund of the Republic of Serbia, Green program of cooperation between science and industry, grant no. 5661, project acronym – IonCleanTech. Any opinions, findings, conclusions or recommendations expressed are those of the authors and do not necessarily reflect the views of the funder.

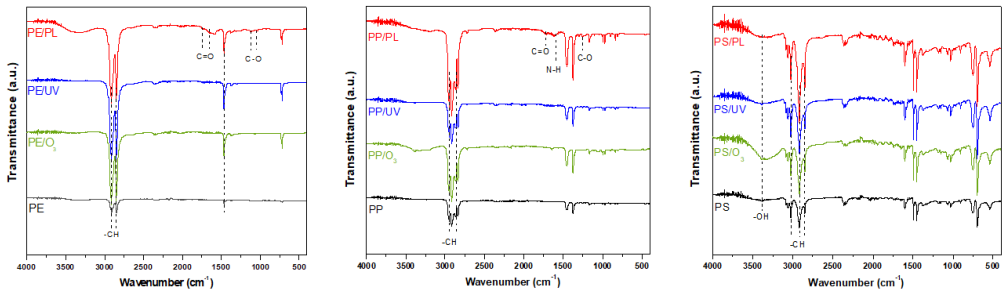

FIGURE 1. FTIR spectra of PE (left), PP (center), and PS (right), without and after the plasma, UV, or O_3 treatment.

REFERENCES

1. Rillig, M.C., Kim, S.W., Kim, T.-Y., Waldman, W.R., *Environ. Sci. Technol*. **55**(5), 2717-2719 (2021).
2. Ćurčić, M., Kolarž, P., Hadžić, B., Stajčić, I., Maletić, D., Aničić Urošević, M., Ilić, A., "Plasma, UV radiation and ozone for microplastics degradation: Optical characterization of polystyrene, polyethylene and polypropylene degradation using FTIR and Raman spectroscopy," manuscript under review.
3. Prata, J.C., Reis, V., Matos, J.T.V., da Costa, J.P., Duarte, A.C., Rocha-Santos, T., *Sci. of the Total Environ.* **690**, 1277-1283 (2019).

Performance Enhancement of HVAC Filters by Unipolar Ionization

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Abstract. Central heating, ventilation, and air-conditioning (HVAC) filtration systems serve for controlling aerosol pollutants in buildings. Although there is an availability of high-efficiency filters, due to the much lower price and less stringent other requirements, the majority of homes and buildings are equipped with much less expensive, low-packing-density fiber HVAC filters, which have low collection efficiency [1]. Fortunately, enhancement of the filtering efficiency of lower-class filters by applying small air ions, along with the decrease of the pressure drop, has been demonstrated for certain pollutants under particular conditions. A continuous emission of unipolar ions has increased the collection efficiency of low-grade HVAC filters challenged with 1 μm PSL particles from 5–15% even up to 40–90% [1]. The effects of different concentrations and exposure times of positive, negative, and bipolar ions have been studied for virus aerosols [2]. A report on the long-term performance of air filters assisted with ionizers has shown the efficiency of the ionizer-assisted synthetic fiber filters to be equal to or higher than the efficiency of a higher class (glass) filter without ionization during more than 6 months [3]. The absence of any associated pressure drop is important, as it means that the efficiency of the filters will be increased without reducing their air-flow due to increased filter density. If the air in front of the filter is intensively ionized, incoming particles will be charged and they will accumulate more actively on the filter. Different airflow rates, distances of ionizers from filters, and filter types, have been used in the above mentioned studies. Here, we review recent investigations in this field and report on the results obtained in our experiments with small air ions and aerosols.
Acknowledgement. This work has been supported by The Science Fund of the Republic of Serbia, Green program of cooperation between science and industry, grant no. 5661, project acronym – IonCleanTech. Any opinions, findings, conclusions or recommendations expressed are those of the authors and do not necessarily reflect the views of the funder.

REFERENCES

1. Agranovski, I.E., Huang, R., Pyankov, O.V., Altman, I.S., Grinshpun, S.A., *Aerosol Sci.Technol.* **40**(11), 963-968 (2006).
2. Hyun, J., Lee, S.G. and Hwang, J., *J. Aerosol Sci*. **107**, 31-40 (2017).
3. Shi, B. and Ekberg, L., *Environ. Sci. Technol*. **49**, 6891-6898 (2015).

Cyst Recognition in Microscopic Slides: Estimation of *Toxoplasma Gondii* Brain Cyst Size and Location

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Abstract. This work describes a recently developed algorithm, performing automatic detection, i.e., recognition, of brain cysts within a tissue homogenate [1]. It is based on fractal dimension (*FD*) as a differentiating parameter, since *FD* was relatively stable for different parasite strains, cyst age, or mice genetic background, and did not change significantly with immunosuppressive treatment or reactivation of latent infection. Additionally, it is convenient to have *FD* already calculated for each cyst which is found. Method is based on a block-based multiscale analysis, employed to identify regions of high-resolution microscopic images which can be classified as *T. gondii* brain cysts. Several sweeps of entire digitalized slides are typically sufficient to statistically determine the brain cyst locations and sizes. The performance estimates are shown for several examples.
Acknowledgement. This work was supported by the Science Fund of the Republic of Serbia through the PRIZMA Research Program (Project No: 7328, Project acronym: ToxoReTREAT).

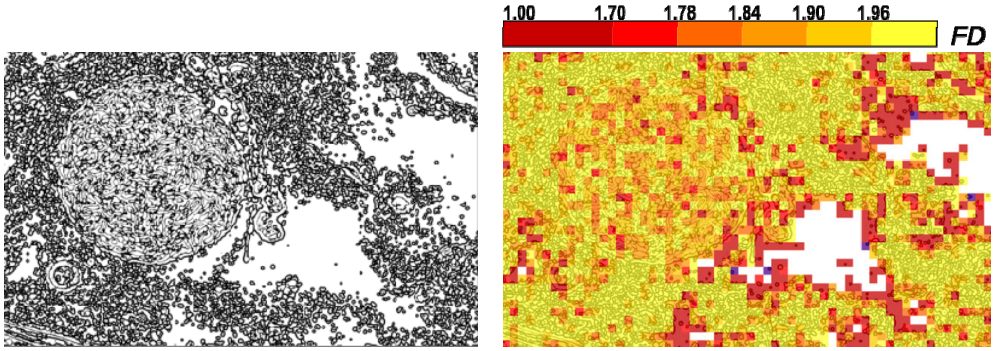

FIGURE 1. High resolution microscopic image of a *T. gondii* brain cyst upon applied threshold and binarization (left). Fractal dimension obtained in a block-based analysis with the block size 40 px [1] (right).

REFERENCES

1. Ilić, A.Ž., Trajković, J., Srbljanović, J., *et al*., "Development of an algorithm for recognition of *T. gondii* brain cysts in microscopic images based on fractal dimension," submitted to *Eur. Phys. J. ST* (2024).

Intercalated $ZrTe_3$ by Fe: A Mössbauer Effect Study

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Abstract. Quasi low dimensional trichalcogenides and dichalcogenides, as well as rare-earth tritellurides are metals with anisotropic electronic structure and charge density wave order [1]. $ZrTe_3$ is a quasi-1D conductor where charge density wave and superconducting quantum states arise due to Fermi surface instabilities and electron-phonon coupling [2]. These physical characteristics classify $ZrTe_3$ as a charge density wave superconductor [3]. There is an interest to reveal how the charge density waves react to changes caused by chemical pressure and local structure distortion due to incorporation of a transition metal ion [4]. The goal of this work is to provide an insight into hyperfine interactions in the Fe^{57}-Mössbauer spectrum in $Fe_{0.1}ZrTe_3$ calculated by the *Vienna Ab-initio Simulation Package*. The lowest defect formation energy was obtained for the interstitial position of Fe ion within the van der Waals gap. I will discuss the impact of the local structural distortion on the ground electronic state.

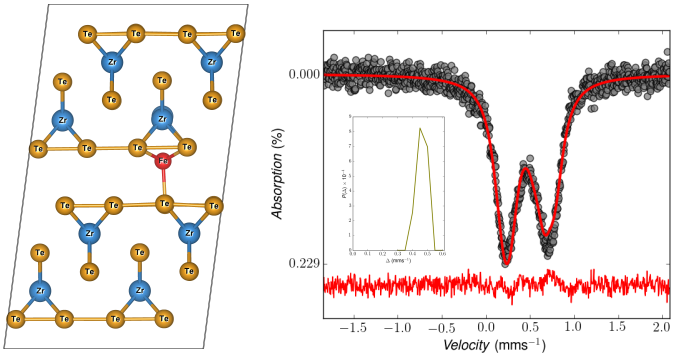

FIGURE 1. The $a-c$ plane of $Zr_{16}Te_{48}Fe$ crystal compound (left). The Mössbauer spectrum obtained on the $ZrTe_3Fe_{0.1}$ sample. The inset shows the quadrupole splitting distribution (right).

REFERENCES

1. Hoesch, M., Cui, X., Shimada, K., Battaglia, C. Fujimori, S., and Berger, H., *PHYS REV B* **80**, 075423-8 (2009).
2. Hu, Y., Zheng, F., Ren, X., Feng, J., and Li, Y., *PHYS REV B* **91**, 144502-10 (2015).
3. Gleason, S. L., Gim, Y., Byrum, T., Kogar, A., Abbamonte, P., Fradkin, E., MacDougall, G. J., Van Harlingen, D. J., Zhu, Xiangde, Petrovic, C., and Cooper, S. L., *PHYS REV B* **91**, 155124-6 (2015).
4. Ganose, A. M., Gannon, l., Fabrizi, F., Nowell, H., Barnett, S. A., Lei, Hechang, Zhu, Xiangde, Petrovic, C., Scanlon, D. O., and Hoesch, M., *PHYS REV B* **97**, 155103-10 (2018).

Future Research Opportunities at European Spallation Source

Andrew Jackson

European Spallation Source, Lund, Sweden

Abstract. The European Spallation Source (ESS) is a multi-disciplinary research facility based on the world's most powerful neutron source with a vision to enable scientific breakthroughs in research related to materials, energy, health, and the environment, and address some of the most important societal challenges of our time. It is currently being built in Lund, Sweden. The initial suite of neutron instruments will consist of 15 instruments, covering a wide range of elastic and inelastic neutron scattering techniques. Each of the instruments has a unique design and targets specific scientific user communities around the world. Taking advantage of the brightness of the ESS source and the use of cold and thermal neutron moderators, these instruments will open new frontiers in time-of-flight neutron powder diffraction, engineering diffraction, single-crystal diffraction with polarized neutrons, and macromolecular crystallography. In this talk, I will provide a brief overview of those instruments and the current status of the ESS project. I will also introduce the methodology behind time-of-flight neutron diffraction and present several examples. Finally, I will discuss our plans for the transition of ESS into user operations and future research opportunities.

REFERENCES

1. Andersen, K.H et al., "The instrument suite of the European Spallation Source", Nuclear Inst. and Methods in Physics Research, A **957**, 163402 (2020).

Respiratory Infections Of Viral Etiology In Immunosuppressed Individuals

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Abstract. Respiratory infections of viral etiology pose a significant threat to immunosuppressed individuals, often leading to severe complications and increased mortality [1]. Key pathogens include influenza A and B, SARS-CoV-2, respiratory syncytial virus (RSV), rhinoviruses, parainfluenza virus, and human metapneumovirus. Due to atypical presentations and prolonged viral shedding in these patients, early and accurate diagnosis is essential [2]. Molecular methods, such as PCR and multiplex panels, provide rapid and precise identification, improving clinical management. Prevention remains crucial, emphasizing vaccination, antiviral prophylaxis, and strict infection control measures. Monitoring viral epidemiology and outbreaks, promptly screening symptomatic patients, and enforcing strict infection control in both outpatient and inpatient settings are crucial to protecting high-risk individuals from viral spread [3].

Acknowledgement. This work has been supported by The Science Fund of the Republic of Serbia, Green program of cooperation between science and industry, grant no. 5661, project acronym – IonCleanTech. Any opinions, findings, conclusions or recommendations expressed are those of the authors and do not necessarily reflect the views of the funder.

FIGURE 1. The timeline of viral infections: past, present and future – courtesy of ChatGPT.

REFERENCES

1. CDC. Respiratory Viruses and People with Weakened Immune Systems. Available on: https://www.cdc.gov/respiratory-viruses/risk-factors/weakened-immune-systems.html
2. Couch RB, Englund JA, Whimbey E. Respiratory viral infections in immunocompetent and immunocompromised persons. *Am J Med*. 1997 Mar 17;102(3A):2-9; discussion 25-6. doi: 10.1016/s0002-9343(97)00003-x
3. Englund J, Feuchtinger T, Ljungman P. Viral infections in immunocompromised patients. Biol Blood Marrow Transplant. 2011 Jan;17(1 Suppl):S2-5. doi: 10.1016/j.bbmt.2010.11.008.

Application Of Scientific Methods In Research On Mural Paintings

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Abstract. Technical protection measures on immovable cultural properties can only be undertaken after preliminary investigations using physical-chemical and other methods to determine the materials' chemical composition, manufacturing techniques, condition assessments, and causes of deterioration. This approach is both a legal obligation and a practical necessity to ensure that planned conservation-restoration activities are performed correctly and based on scientific evidence. Research on immovable cultural properties encompasses a broad range of activities; however, this paper focuses on investigative conservation-restoration work that applies precise scientific methods from chemistry and physics to the examination of wall paintings, aiming to enhance conservation practices. Such research involves identifying the materials used, determining the painting techniques, assessing the state of preservation, and establishing the causes of degradation. To achieve this, a variety of physicochemical methods are employed to analyze different samples constituting the monument. This includes examining various construction materials, supports, substrates, painted layers, gilding, mosaics, icons, and other artistic objects. Analysis focuses on identifying binding agents and their origins, conducting cleaning tests, and formulating agents for removing varnishes, coatings, and other deposits and impurities. Additionally, qualitative elemental analysis, salt presence analysis, and sample microscopy are performed. A significant aspect of the research also involves monitoring the microclimatic conditions surrounding the monument and investigating the sources and origins of moisture. A case study of the Church of the Holy Trinity in the Sopoćani Monastery illustrates the methodology and systematic approach of these research activities. Based on research findings, measures were implemented to improve the site's condition and execute conservation treatments, following project development.

Material Science using MAX IV – the First 4th Generation Synchrotron Source

Mads Ry Vogel Jørgensen[a, b]

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Abstract. MAX IV Laboratory is Sweden's national synchrotron radiation facility, home to three accelerators with distinct characteristics [1, 2]. Among them, the 3 GeV storage ring stands out as the world's first fourth-generation synchrotron, pioneering the multibend achromat lattice to deliver ultrahigh-brightness X-rays. The facility currently operates 16 beamlines, supporting a wide range of experimental techniques. In this presentation, I will provide an overview of MAX IV and its beamlines, with a particular focus on those at the 3 GeV storage ring. I will highlight the DanMAX beamline, designed for materials science through powder X-ray diffraction, total scattering, and full-field imaging, and I will present examples of how we've used scanning diffraction to resolve atomic structures with high spatial resolution.

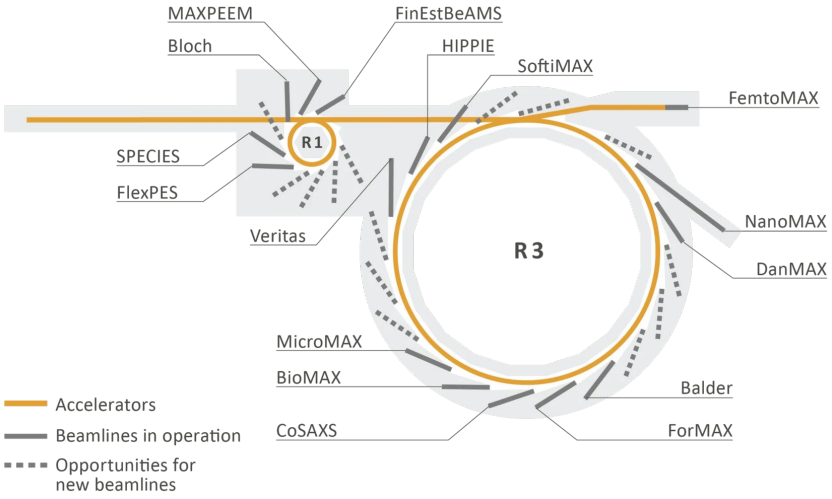

FIGURE 1. Overview of the MAX IV accelerators and beamlines.

REFERENCES

1. Tavares, P. F., Al-Dmour, E., Andersson, Å., *et al*., J. Synchrotron Rad. **25**, 1291-1316 (2018).
2. Robert, A., Cerenius, Y., Tavares, P. F., *et al.*, Eur. Phys. J. 138, 495 (2023)

Electronically-Driven Local Lattice Distortions in Molecule-Intercalated Iron-Chalcogenide Superconductors

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Abstract. The origin of unconventional high-T_c superconductivity in iron chalcogenides (Fe*Ch*s) remains highly puzzling due to their multiorbital nature, which drives intertwined anisotropic spin, orbital, and structural instabilities. [1,2] To determine which instability primarily influences superconductivity, we investigate analogous electron-correlation-driven instabilities in newly synthesized high-T_c $Li_x(C_5H_5N)_yFe_{2-z}Se_2$ derivatives (Fig. 1a, b; right motifs). In these *2D* systems, the local $FeSe_4$ geometry is a key factor in their electronic properties. [3,4] Complementary synchrotron diffraction and spectroscopic studies investigate subtle structural and electronic modifications and their relation to superconductivity. Structural analysis reveals that $FeSe_4$ tetrahedra adopt an ideal geometry (inset; Fig. 1a), suppressing orbital differentiation under Hund's rules and inducing anisotropic electronic instabilities. While the one system exhibits a nematic distortion (*Pnma*), which is suppressed below T_c, the other one adopts a tetragonal (*I4/mmm*) lattice, where negative thermal expansion (NTE) in the Fe-Fe network evolves below T_c (Fig. 1c, d). Thermal expansion coefficients (Fig. 1e, f) confirm that these structural instabilities stem from electronic anisotropies. X-ray emission spectroscopy (XES) links NTE to an increased Fe 3*d* local spin moment due to selective localization of d_{xy} under Hund's rules (Fig. 1g). This suggests that local magnetic fluctuations likely play a dominant role in superconductivity over nematic ones. Understanding the pairing mechanism is key to designing higher-T_c Fe*Ch*s.

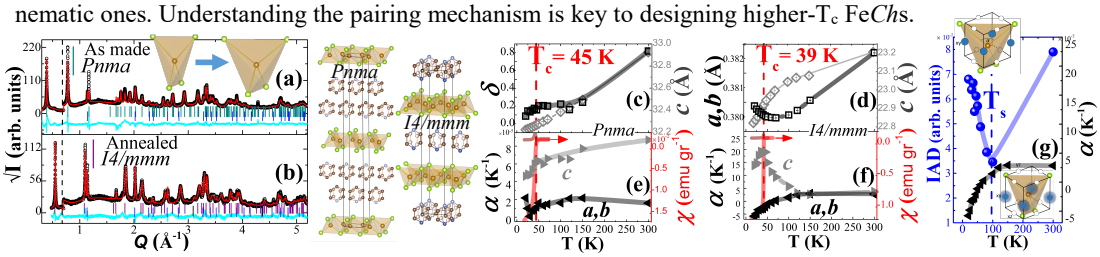

FIGURE 1. (a), (b) Rietveld fits, (c), (d) unit cell parameters, (e), (f) TECs, (g) Fe Kβ XES IAD vs TEC.

REFERENCES

[1] D. J. Scalapino, Rev. Mod. Phys. **84**, 1383 (2012). [2] S. M. Souliou, *et al*., Synchrotron Radiat. News **36**, 3 (2023). [3] A. Deltsidis, *et al*., Inorg. Chem. **61**, 12797 (2022). [4] M. Yi, Y. Zhang, *et al*., Npj Quantum Mater. **2**, 1 (2017).

Novel 2D Hybrid Platforms for Emerging Applications

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Abstract. Nanoscience and Nanotechnology research has made significant contributions addressing issues related to energy, water, food and health security. Hybrid nanostructures are found to be much more promising as we can integrate the properties of the constituents and achieve synergetic effects. Among various nanostructures, 2D materials are very promising to engineer SERS platforms with Ag and/Au nanoparticles. Surface Enhanced Raman Spectroscopy (SERS) is an ultrasensitive method for the detection of different analytes present in traces or even single molecule levels by the generation of electromagnetic fields. It is an extremely powerful vibrational spectroscopic method that is capable to detect traces of chemical and biological analytes. In the vicinity of nanomaterials decorated surfaces, SERS can monitor extremely low concentrations of analytes in a non-destructive manner with narrow line widths. In order to address the present energy crisis, hydrogen is considered as an efficient alternative for the energy requirements. Different materials have been developed over the years for hydrogen production. This talk will cover our recent works on novel engineered Graphene, TMDCs and MXene based hybrid structures for SERS detection of emerging pollutants and electro-catalysis for water splitting.

Coexistence of Superconductivity and Chiral Charge Density Wave in $TiSe_2$

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Abstract. Chirality breaks down the inversion symmetry and results in unexpected new electronic properties in systems with reduced dimensionality. Stark examples of manifestation of chirality on electronic properties of materials are carbon nanotubes. In addition to structural chirality, the chiral state can also manifest itself in the arrangement of electronic states – magnetic vortices, skyrmions, chiral superconductors. $TiSe_2$ is the first known transition metal dichalcogenide that exhibits chiral charge density wave state.

We demonstrate the chiral properties of the CDW through several independent techniques: scanning probe microscopy, transient optical reflectivity and photogalvanic effect. As temperature is decreased below T_{CDW}=200 K 1T-$TiSe_2$ goes first from the high temperature normal phase to a 2 × 2 × 2 achiral CDW phase at T_{CDW} and then to a chiral phase at T_{ch}. These two thermodynamic transitions were first observed using bulk thermodynamic techniques [1], and their nature explored in more detail using photogalvanic effect [2]. The structure of the chiral CDW was imaged using scanning tunneling microscopy [3], while time-resolved optical reflectivity and IR studies clearly show that the chiral order can be non-thermally melted and controlled using circularly polarized light. Further studies using X-ray photon correlation spectroscopy show that the charge density wave has distinct dynamics near the transition temperature.

Our study provides compelling evidence for the spontaneous emergence of chirality in the correlated semimetal $TiSe_2$. Such chiral induction provides a new way of optical control over novel orders in quantum materials and potential for novel electrooptical sensing.

REFERENCES

1. J.-P. Castellan, S. Rosenkranz, R. Osborn, Q. Li, K. E. Gray, X. Luo, U. Welp, G. Karapetrov, J. P. C. Ruff, & J. van Wezel, *Phys.Rev.Lett*, **110** 196404 (2013).
2. S.-Y. Xu, Q. Ma, Y. Gao, A. Kogar, G. Zong, A. M. M. Valdivia, T. H. Dinh, S.-M. Huang, B. Singh, C.-H. Hsu, T.-R. Chang, J. P. C. Ruff, K. Watanabe, T. Taniguchi, T.-R. Chang, H. Lin, G. Karapetrov, D. Xiao, P. Jarillo-Herrero, & N. Gedik, *Nature* **578** 545 (2020)
3. M. Iavarone, R. Di Capua, X. Zhang, M. Golalikhani, S. A. Moore, & G. Karapetrov, *Physical Review B*, **85** 155103 (2012).

Ultra-thin ZnO Coatings on Microstructured γ-Fe_2O_3 Thin Films Prepared by Atomic Layer Deposition for Enhanced Photocatalysis

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Abstract. Water pollution from industrial activities and organic contaminants remains a pressing environmental challenge, necessitating innovative and effective solutions [1]. Among these, photocatalytic degradation has emerged as a promising method for breaking down pollutants into harmless by-products like carbon dioxide and water by utilizing light energy and semiconductor materials [2]. A key factor in optimizing this process is increasing the surface-to-volume ratio, which enhances photocatalytic efficiency by maximizing the number of active sites available for pollutant degradation, leading to faster and more effective reactions [3]. This research explores the photocatalytic efficiency of ultra-thin ZnO layers deposited on γ-Fe_2O_3 microstructured films through atomic layer deposition. To create these films, rod-like silica-coated γ-Fe_2O_3-SiO_2 core-shell microparticles of varying sizes and silica layer thicknesses were assembled using the drop-casting method. The deposition rate of ZnO was found to be closely linked to the concentration of hydroxyl (-OH) functional groups on the γ-Fe_2O_3 surface. Various analytical techniques, including scanning electron microscopy, transmission electron microscopy, atomic force microscopy, and X-ray photoelectron spectroscopy, were employed to examine the surface morphology, roughness, and chemical composition of the microstructured ZnO coatings. The photocatalytic performance of the samples was assessed by measuring the degradation of methylene blue in an aqueous solution under UV light exposure. The most active γ-Fe_2O_3-ZnO sample exhibited a photodegradation rate approximately three times greater than that of a reference ZnO film on a silicon substrate. A strong relationship was observed between photocatalytic efficiency and the surface roughness and morphology of the γ-Fe_2O_3 microstructured films. Higher photocatalytic activity was recorded for γ-Fe2O3-ZnO samples that maintained the original structure of the γ-Fe_2O_3 films after ZnO deposition while exhibiting increased surface roughness. These findings

highlight the potential of ultra-thin ZnO coatings on microstructured γ-Fe_2O_3 films for environmental applications, particularly in the degradation of pollutants in water.

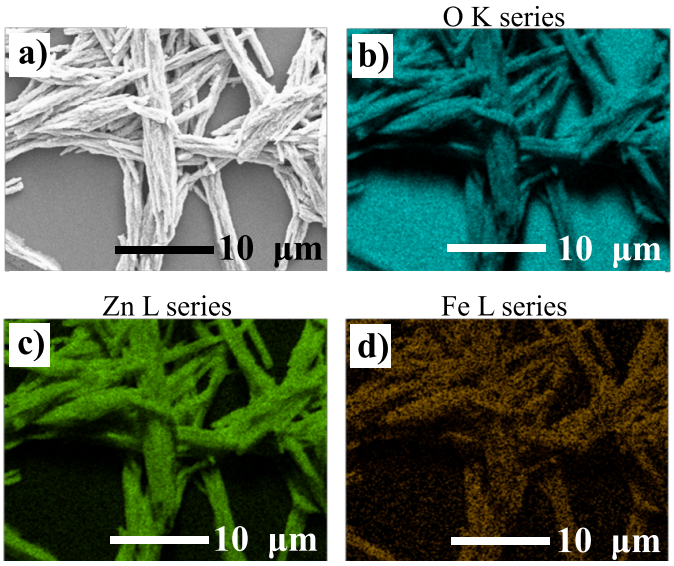

FIGURE 1. SEM image a) and EDS maps of O K series b), Zn L series c) and Fe L series d) of the γ-Fe_2O_3 microparticles coated with ALD ZnO film.

REFERENCES

1. Fuzil, N. S., Othman, N. H., Alias, N. H., Marpani, F., Othman, M. H. D., Ismail, A. F., Lau, W. J., Li, K., Kusworo, T. D., Ichinose, I. et al., *Desalination* **517**, 115259 (2021).
2. Kisch, H., Semiconductor Photocatalysis: Principles and Applications, *Wiley-VCH: Weinheim* 2015.
3. Zeid, S. A., Leprince-Wang, Y., *Crystals* **14**, 611 (2024).

Experimental Methods for Investigation of Ion-Aerosol Interaction

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Abstract. The main objective of the IonCleanTech project is to utilize the potential of ozone-free ionization to deposit and neutralize air pollutants, nonbiological as well as biological, in the breathing zone in indoor spaces. The presence of particulate matter (PM) as well as volatile organic compounds (VOCs) in indoor air is a sustained problem of public health in modern societies. In addition to the acquired equipment for precise aerosol concentration measurements, we have devised and custom-built the exposure systems to improve experimental accuracy and facilitate the interaction of small air ions with bioaerosols, despite sometimes limited quantities of pathogens constituting the bioaerosol. We have conducted elaborate analyses for a wide range of pollutants under laboratory as well as real-life conditions [1]. The obtained results are important as a starting point for the most efficient ion-rich air delivery into the air breathing zone.
Acknowledgement. This work has been supported by The Science Fund of Serbia, Green program of cooperation between science and industry, grant no. 5661, project acronym IonCleanTech.

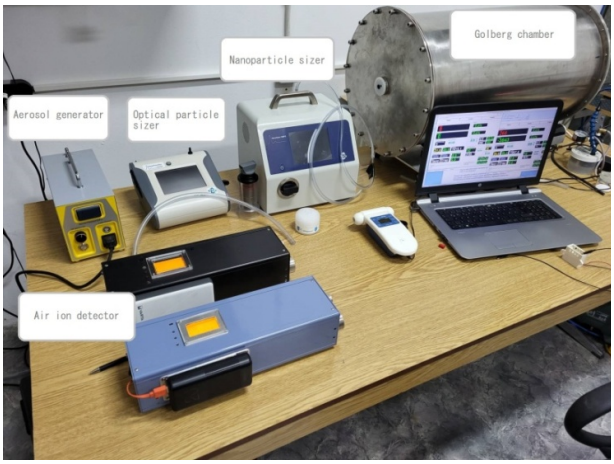

FIGURE 1. Aerosol and ion generation equipment, ozone level monitoring, aerosol particle concentration and ion concentration measurement equipment.

REFERENCES

1. Kolarž, P., Ilić, A.Ž., Janković, M., Janićijević, A., Trbovich, A.M., *J Aerosol Sci*. **173**, 106199 (2023).

Removal and Inactivation of Bacteria and Fungi by Ionization

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Abstract. Generally, small air ions have been shown to electrostatically enhance the deposition of airborne particles in indoor air, an effect closely linked to the particle size [1]. Additionally, air ions have been reported to produce a biocidal action on airborne microorganisms [2], [3]. We report on the results of exposure of bacteria and fungi to negativelly charged ions of varying concentrations for different time durations. Significant effects were observed in either eliminating the microorganisms or impacting colony morphology and, in case of fungi, spore germination dynamics. Hence, air ions offer the possibility to reduce the amounts of airborne pathogens.
Acknowledgement. This work has been supported by The Science Fund of Serbia, Green program of cooperation between science and industry, grant no. 5661, project acronym IonCleanTech.

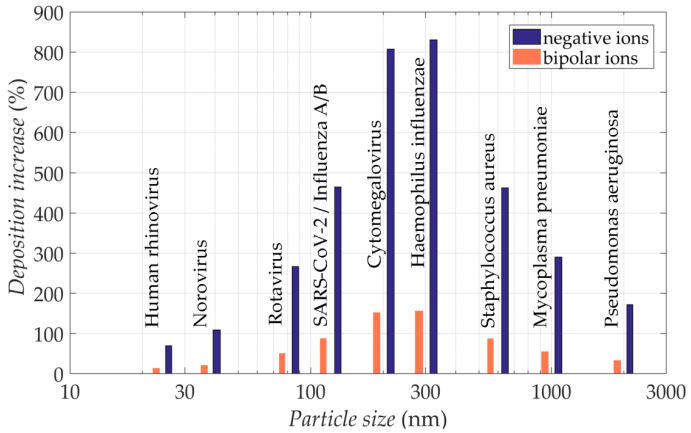

FIGURE 1. Estimates of possible efficiency of small air ions in increasing the particle deposition rates, based on experiments with NaCl particles of different sizes. (Please see [1],[2]).

REFERENCES

1. Kolarž, P., Ilić, A.Ž., Janković, M., Janićijević, A., Trbovich, A.M., *J Aerosol Sci*. **173**, 106199 (2023).
2. Fletcher, L.A., Gaunt, L.F., Beggs, C.B., *et al.*, *BMC Microbiology* **7**, 32 (2007).
2. Radalj, A., Nikšić, A., Trajković, J., *et al.*, *Appl. Sci*. **14**(16), 7311 (2024).

Nanostructured thin films with strong spin-orbit interaction

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Abstract. Materials with strong spin-orbit coupling (SOC) position themselves at the frontline of spintronics, allowing generation and manipulation of pure spin-currents [1]. Perovskite iridates have received special interest as they exhibit a rich electronic phase diagram with exotic states, due to the delicate interplay between SOC and crystal field splitting. In particular, $SrIrO_3$ has been proposed as a topological semimetal, having band structures near the transition between semi-metallic and insulating states, which can be finely tuned by strain and deposition conditions [2]. This electronic richness mixed with the inherent tendency of perovskite oxides towards self-organized growth offers an enormous and unexplored potential for engineering functional properties of thin films [3]. The influence of strain and nanostructured formation at the surface on electronic transport properties of $SrIrO_3$ is discussed (Figure 1).

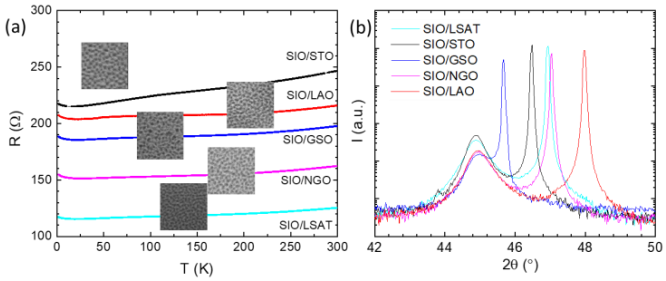

FIGURE 1. (a) Temperature dependent resistance of nanostructured $SrIrO_3$ thin films grown on different substrates ($SrTiO_3$ (STO), $LaAlO_3$ (LAO), $NdGdO_3$ (NGO), $GdScO_3$ (GSO), $(LaAlO_3)_{0.3}$–$(Sr_2AlTaO_6)_{0.7}$ (LSAT) with SEM images (2x2 μm^2) (b) θ-2θ measurements of the corresponding films with similar thickness (25 nm<t<30 nm).

REFERENCES

1. Martin-Rio, S. et al., *ACS Applied Materials and Interfaces* **15**, 37038-37046 (2023).
2. V. Fuentes et al., *Nanomaterials* **14**, 242 (2024).
3. Konstantinović, Z. et al., *Small* **5**, 265 (2009); Konstantinović, Z. et al., *JMMM* **509**, 166898 (2020).

Advances in IMD Processed MgB_2 Wires for Potential Applications

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Abstract. MgB_2 superconducting wires have emerged as a promising candidate for practical applications due to their relatively low cryogenic cooling requirements and material costs, offering efficient operation around 20 K. Two major fabrication methods are commonly employed for MgB_2 wire production: the Powder-In-Tube (PIT) method and the Internal Mg Diffusion (IMD) method. Wires produced via both approaches typically exhibit a high-density MgB_2 phase with improved grain connectivity, which contributes to enhanced transport critical current density (Jc). While the PIT method has been widely investigated over the past two decades with several achievements, the IMD technique has recently gained increased attention due to its potential to improve structural uniformity and increase the MgB_2 fill factor. This study presents recent advancements in the fabrication of IMD-processed MgB_2 wires, focusing particularly on the effects of copper coating and carbon doping strategies for performance enhancement. Application-specific Jc requirements vary significantly: for MRI magnets, high Jc values at moderate magnetic fields (1–3 T) are essential to ensure stable and homogeneous field generation; in contrast, fusion and high-field research magnets require robust Jc performance in fields exceeding 5 T. Furthermore, applications such as power transmission lines and fault current limiters demand thermally stable conductors with long-term current-carrying capability. Our results demonstrate that wires produced using Cu-coated Mg rods and carbon-doped boron precursors exhibit improved microstructural homogeneity, enhanced flux pinning, and refined grain boundary properties, enabling high Jc values under a wide range of operating conditions. Additionally, Turkiye's substantial reserves of high-purity boron have enabled the successful domestic production of amorphous boron powders, contributing significantly to the development of MgB_2 wire technology. These findings highlight the strong potential of IMD-processed MgB_2 wires, especially when optimized through doping, coating, and processing techniques, to meet the diverse demands of modern superconducting applications.

This work has been supported by TÜBİTAK and Chinese Academy of Sciences (CAS) via Bilateral Cooperation under contract No: 123N624

Exploring New Horizons: Epitaxial Growth of Next-Generation 2D Materials

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Abstract. Long before graphene gained fame in 2004 [1], its epitaxial growth was realized in surface science studies focused on the adsorption and decomposition of hydrocarbons on metal substrates [2]. The surface parameters play a crucial role in the synthesis of various two-dimensional (2D) materials, including graphene, transition metal dichalcogenides (TMDs), and novel homoelemental materials. The broad parameter space for the growth is influenced by factors such as surface chemical reactivity, lattice parameters, anisotropy, surface alloying, and more. In this talk, I will present recent examples of research conducted by the *Surfaces, Interfaces and 2D Materials* research group in Zagreb. The focus will be on several examples of epitaxially grown atomically thin 2D materials and heterostructures with potential for novel applications. These examples highlight the unique properties of 2D materials and heterostructures. In the case of 2D borophene (Bo), we have developed novel in-situ and ex-situ growth, characterization, and manipulation methods. Specifically, X-ray photoelectron spectroscopy (XPS) and scanning tunneling spectroscopy (STS) data reveal inhomogeneous binding of Bo to Ir, resulting in a stripe-like structure. This structure acts as a one-dimensional grating, inducing Umklapp scattering of photoelectrons detected in ARPES experiments [3]. Furthermore, our results demonstrate that ex-situ deterministic manipulation of Bo layers is feasible despite their inherent chemical and mechanical instability, advancing Bo research and utilization [4]. We will also address TMD-graphene heterostructures. Our goal was to achieve quasi-freestanding TMD systems and characterize the effects of vertical and lateral stacking of MoS_2 and WS_2 [5]. Additionally, we explored how intentional self-intercalation during growth enables efficient in-situ chemical and physical engineering of material properties, particularly the electronic band-structure [6].

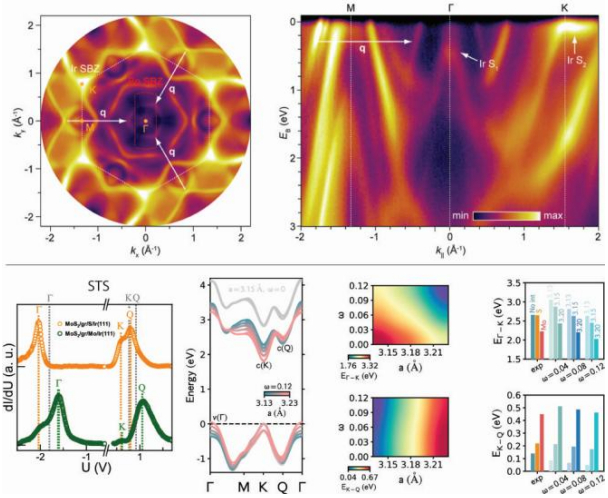

FIGURE 1. Examples of ARPES characterization of Bo [3] (upper panel), and in the lower panel STS characterization of modified MoS_2 via self-intecalation, with corresponding theoretical model [6].

REFERENCES

1. Novoselov, K.S., Geim, A.K., Morozov, S.V., Jiang, D. et al., *Science* **306**, 666-669 (2004).
2. Land, T.A., Michely, T., Behm, R.J., Hemminger, J.C., Comsa, G., *Surf. Sci.* **264**, 261-270 (1992).
3. Kamal, S., Seo, I., Bampoulis, P., Jugovac, M., et al., *ACS Appl. Mater. Interfaces* **15**, 57890–57900 (2023).
4. Radatović, B., Jadriško, V., Kamal, S., Kralj, M., et al., M., *ACS Appl. Mater. Interfaces* **14**, 21727–21737 (2022).
5. Pielić, B., Novko, D., Šrut Rakić, I., Cai, J., et al., *ACS Appl. Mater. Interfaces* **13**, 50552–50563 (2021).
6. Pielić, B., Mužević, M., Novko, D. Cai, J., et al., *npj 2D Mater. Appl.* **8**, 61 (2024).

Physical Characterization and Device Application of Organic Bilayer Films

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Abstract. Flexible sensors made from organic bilayer films of molecular conductor on polymeric matrix have attracted many interest due to their simple fabrication with high potential for being scaled up, and for their high-performing multi-functionality at room temperatures. In particular, the piezoresistive property of the organic bilayer film is among one of the highest ever reported, allowing its utilization in various sensing applications. The study of the flexural piezoresistivity of an organic bilayer film based on β−(BEDT−TTF)$_2$I$_3$ on polycarbonate matrix from room temperatures down to cryogenics temperatures is presented. Due to the introduced disorder in the film, non-trivial temperature dependent profile of the gauge factor is revealed, including enhancement of the gauge factor from ∼18 at room temperatures to ∼48 at 4.3 K. The organic bilayer cantilever magnetometer is developed and demonstrated to measure magnetic properties of a single crystalline organic superconductor κ−(BEDT−TTF)$_2$Cu(N(CN)$_2$)Br at cryogenic temperatures down to ∼2.75 K and magnetic fields up to 5 T. The high-performing bilayer devices can be fabricated in a very simple manner, and they are robust and recyclable. It is also used for performing simultaneous torque-transport measurements of both the layered perovskite superconductor Sr_2RuO_4 and layered organic superconductor κ−(BEDT−TTF)$_2$Cu(NCS)$_2$. The measurements performed on the same sample enable observation and determination of the phase shift between magnetic quantum oscillations of the magnetization and magnetoresistance.

REFERENCES

1. E. Steven, D. Krstovska, D. Suarez, T. Berliani, E. Jobiliong, E. S. Choi, Sensors and Actuators A: Physical, 368 (2024)

Universal low-temperature fluctuation of unconventional superconductors revealed

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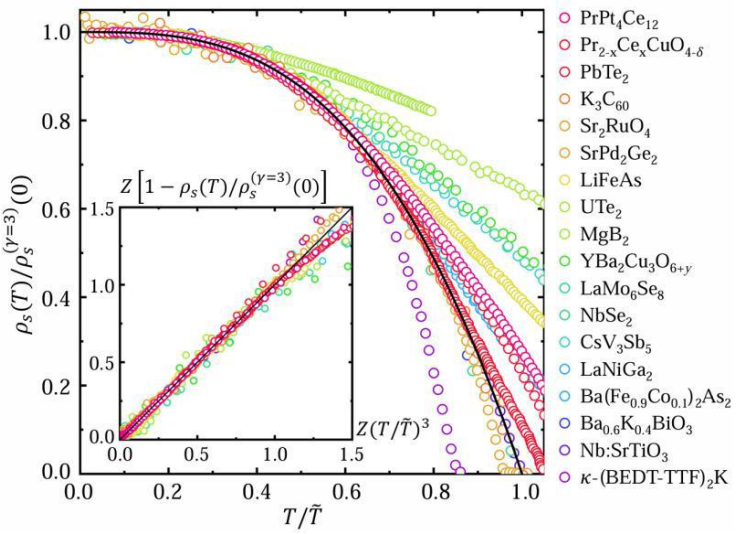
Abstract. Low-temperature thermal fluctuations offer an essential window in characterizing the true nature of a quantum state of matter, a quintessential example being Fermi liquid theory. In the long-standing pursuit toward a fundamental understanding of unconventional superconductivity, the most essential low-temperature thermal fluctuation of superfluidity has unfortunately been greatly overlooked. Here, we examine the leading thermal fluctuation of the superfluid density across numerous families ranging from relatively conventional to highly unconventional superconductors (MgB_2, bismuthates, doped buckyballs, heavy fermions, UTe_2, doped $SrTiO_3$, Chevrel clusters, intermetallics, κ-organics, transition metal dichalcogenides, ruthenates, iron-pnictides, cuprates, and kagome metals). Amazingly, in all of them an unprecedented universal T^3 depletion materializes in the low-temperature superfluid density, even in the believed-to-be-conventional MgB_2. This reveals a new quantum superfluid state of matter and requires a necessary change of paradigm in describing modern superconductors. We demonstrate that such unorthodox yet generic behavior can be described by a Galilean invariant theory of bosonic superfluidity hosting a long-lived `true condensate'.



REFERENCES

1. Anthony Hegg et al, arxiv.org/abs/2402.08730.
2. Anthony Hegg, Jinning Hou and Wei Ku, PNAS 118 (46) e2100545118 (2021).
3. Y. Yildirim and Wei Ku, Phys. Rev. X 1, 011011 (2011).

Fluctuating Magnetic Moments Near Superconductivity in Interlayer-Expanded FeSe

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Abstract. The role of correlation-driven instabilities [1] near superconductivity remains debated in multiorbital pairing mechanisms of iron-based superconductors [2]. This study investigates $Li_x(C_5H_5N)_yFe_{2-z}Se_2$, a β-FeSe intercalate with expanded Fe layer spacing (~11.2 Å) [3]. Synchrotron X-ray diffraction and site-selective core-level spectroscopy reveal spontaneous structural distortions. At the global level, negative thermal expansion (NTE) in the 2D Fe network emerges below T_S (~70 K), with strong in-plane microscopic strain. Additionally, changes in local bond dynamics upon cooling across T_c (~39 K) suggest local-mode hardening, indicating that strain in the Se-Fe-Se planes affects lattice fluctuations. Intercalation causes the Se-Fe-Se layer to become thinner, leading to compressed $FeSe_4$ tetrahedra (anion height: 1.455 Å) and moderate electron correlations. As the superconducting state is approached, incoherent $FeSe_4$ atomic rearrangements, modify orbital occupancies and induce site-local fluctuations. In support to this, Fe Kβ X-ray emission spectroscopy detects fluctuating (~10^{-15} s) local spin moments that persist below T_S, in contrast to the Fe-3*d* local moment quenching [4] in related superconductors. The combined analyses suggest that NTE is linked to weak electronic anisotropy, driven by selective localization of in-plane d_{xy} orbitals. This behavior is interpreted as a hallmark of orbital differentiation caused by Hund's coupling-induced orbital-selective electronic correlations. The work underscores how intercalation-mediated adjustments in Fe-3*d* orbital involvement moderate correlation-driven orbital differentiation, offering a pathway to optimize T_c in unconventional superconductors with long interlayer separations.

REFERENCES

1. de' Medici, L., "Weak and Strong Correlations in Fe Superconductors", in *Iron-Based Superconductivity*, edited by P. D. Johnson, G. Xu, and W.-G. Yin, Publisher: Springer Series in Materials Science, vol 211. Springer, Cham., 2015, pp. 409–441.
2. Chubukov, A., *Annu. Rev. Condens. Matter Phys.* **3**, 57-92 (2012).
3. Deltsidis, A., Kaitatzi, M., Simonelli, L., Stock, C., Voneshen, D., and Lappas, A., *Phys. Rev. Mater.* **9**, 024801-11 (2025).
4. Mannella, N., *J. Phys. Condens. Matter* **26**, 473202 (2014).

Exploring Structural Phase Transitions in Atorvastatin Calcium Trihydrate Through Variable-Temperature Raman Spectroscopy

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Abstract. A detailed Raman spectroscopic analysis of atorvastatin calcium trihydrate (Form I) was conducted across a broad temperature range (100 K to 460 K), with particular focus on the low-frequency vibrational region. This study reveals new insights into the structural evolution and thermal response of the compound.

Significant spectral changes were observed near 420 K, where the disappearance of external vibrational modes at ~34 cm^{-1}, 44 cm^{-1} and 140 cm^{-1} indicated a structural phase transition. At the same time, pronounced broadening of the 645 cm^{-1} and 1650 cm^{-1} modes indicated increased molecular fluctuations. A new Raman feature emerging around 75 cm^{-1} during this transition suggests the presence of a transient, ordered intermediate phase before complete loss of crystallinity at higher temperatures.

These findings offer the first in-depth view of temperature-driven structural changes in atorvastatin calcium trihydrate by means of inelastic light scattering, providing valuable information on its vibrational properties, phase behavior and implications for pharmaceutical stability.

Innovative Approach to Studying the Structural, Magnetic and Electrical Characteristics of Nano Spinel Ferrites Prepared via Soft Mechanochemical Synthesis

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Abstract. Ferrites are widely recognized for their valuable combination of ferrimagnetic and electrically insulating properties, making them highly suitable for various technological applications. The crystal structure of spinel ferrites allows for the incorporation of different cations at specific lattice positions, resulting in a broad range of electrical and magnetic characteristics [1]. In this study, spinel ferrites with the general formula $\boldsymbol{M}Fe_2O_4$ ($\boldsymbol{M}$ = Ni, Zn) were synthesized through a soft mechanochemical process using a planetary ball mill. A carefully selected combination of oxides and hydroxides was used as the starting material. This mixture underwent mechanical activation, followed by uniaxial pressing and sintering at 1100°C for 2h. The structural composition of the sintered samples was characterized using XRD, Raman spectroscopy (FIG. 1), and infrared spectroscopy, while their morphology was examined via scanning electron microscopy. The Mössbauer spectra of samples were fitted by several subspectra, and the degrees of inversion were calculated. To assess the electrical properties, DC resistivity measurements were performed across a temperature range of 298-473 K, allowing for the calculation of activation energy. AC conductivity was also investigated within the same temperature range, covering frequencies from 100 Hz to 1 MHz. The results revealed that electrical conductivity increased with rising temperature, confirming the semiconducting nature of the synthesized ferrites. Complex impedance spectroscopy was employed to evaluate the influence of grains and grain boundaries on the overall electrical behavior of the ferrites.

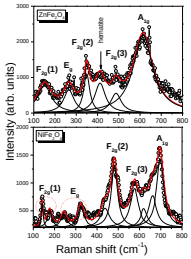

FIGURE 1. Raman spectra of $NiFe_2O_4$ and $ZnFe_2O_4$.

REFERENCES

1. Ahlawat, A., Sathe, V.G., Reddy, V.R., and Gupta, A., *J. Magn. Magn. Mater*. **323**, 2049-2054 (2011).

Can sound be used for time-bin encoding of photonic qubits for secure quantum communication?

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Abstract. Photons excellent carriers of information because they possess several degrees of freedom that can be used to encode data qubits. Currently, most quantum communication protocols are using photon's polarization state to carry a qubit of information by converting it into different photon polarization directions. However, this type of encoding suffers from decoherence via polarization mode dispersion in optical fibers, which hinders its use for long-distance secure quantum communication using the existing telecommunication infrastructure. One way to circumvent this is by employing a different encoding scheme. In this work, we demonstrate progress towards efficient time-bin encoding, via dynamic real-time control, using radio-frequency (RF) surface acoustic waves (SAWs), of the optical emission from quantum dots (QDs) embedded in epitaxially grown core-shell GaN/InGaN nanowire (NW) heterostructures [1]. The SAWs are excited on the surface of a piezoelectric LiNbO3 crystal equipped with an acoustic delay line onto which the NWs were mechanically transferred [2,3]. Luminescent QD-like exciton localization centers, induced by indium content fluctuations within the InGaN nanoshell, are identified as efficient sources of single-photons. These quantum emitters are optically characterized by spatially and polarization resolved micro-photoluminescence as well as photon correlation spectroscopy. Such experiments reveal the appearance of narrow highly linearly polarized emission lines associated with quantum confined exciton (X) and biexciton (XX) exhibiting pronounced photon antibunching [2,3]. When perturbed by the propagating SAW, the NW-QDs are periodically strained and their excitonic transitions are dynamically modulated by the acousto-mechanical coupling, giving rise to spectral fine-tuning of the emitted light within a ~2 meV bandwidth at the acoustic frequency of ~330 MHz. This outcome is further combined with spectrally filtered detection for temporal control of the emitted photons [2]. The stroboscopic measurements performed on our SAW-driven single-photon NW-QD sources under time-resolved detection synchronized with the SAW show weak changes in the emission intensity during the decay of both X and XX luminescence. The amplitude of these oscillations scales with the strength of the SAW piezoelectric field. For sufficiently high acoustic powers resulting in stronger field values, these intensity oscillations become more pronounced making it possible to track their temporal evolution. Their appearance takes place at a well-defined acoustic phase corresponding to the maximum longitudinal SAW piezoelectric field component. We thus relate these oscillations to the field assisted simultaneous transfer into the probed NW-QD emitter of electron and holes which are optically generated in the surrounding InGaN region [3]. The experimentally observed simultaneous injection of the two carrier species into the QD confined energy levels significantly differs from the previous findings reported in other QD systems, in which the SAW-regulated spatio-temporal carrier dynamics leads to preferential sequential carrier injection or extraction [4].

In addition, by employing the acoustic phonon of a specific waveform, the resulting SAW-mediated fine-tuning of the NW-QD emission energy can be combined with spectral filtering to achieve more complex temporal sequence of the emitted photons. In this way, by collecting the light at different energies of the SAW-driven NW-QD spectral response, we are able to control the time sequences of the emitted single photons. Such control of the photon emission or arrival time can be used as a degree of freedom to encode an information qubit on a photon. The advantage of this encoding scheme is its robustness against decoherence, making it better suited for fiber optics applications. Moreover, the observed excitonic complexes suggest that our NW-QD system is promising for achieving still challenging room-temperature production of entangled photon pairs via XX-X radiative cascade. Altogether, this study opens the door to the use of sound for scalable integration of group III-nitride-based quantum emitters in future quantum information technologies.

REFERENCES

1. Ž. Gačević et al., ACS Photon. 4, 657 (2017).
2. S. Lazić et al., Semicond. Sci. Technol. 32, 084002 (2017).
3. S. Lazić et al., J. Phys. D: Appl. Phys. 51, 104001 (2018).
4. O.D.D. Couto et al., Nat. Photonics 3, 645 (2009).

Monitoring of Reactivated Toxoplasmosis in Allogeneic HSCT Recipients

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Abstract. Severe immunosuppression in patients chronically infected with a ubiquitous protozoan *Toxoplasma gondii* can result in reactivated toxoplasmosis (RT), a life-threatening complication, especially for patients undergoing allogeneic hematopoietic stem cell transplantation (HSCT). Activities of the ToxoReTREAT project are focused on the pre-HSCT serological screening and post-HSCT diagnosis of RT, as well as the follow-up on effects of treatment of RT, employing weekly monitoring of peripheral blood samples using an in-house qPCR [1], and an array of serological tests available at the National Reference Laboratory for Toxoplasmosis.
Acknowledgement: This research was funded by the Science Fund of the Republic of Serbia, 7328, Reinvention of the diagnostic algorithm and treatment options for reactivated toxoplasmosis—ToxoReTREAT.

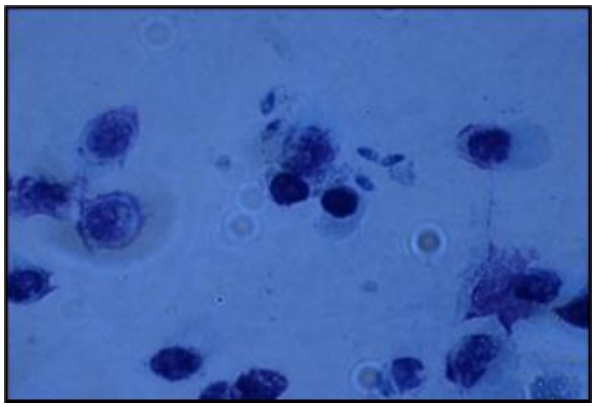

FIGURE 1. *Toxoplasma gondii* tachyzoites on Giemsa-stained bronchoalveolar lavage fluid smears (day 20, post-HSCT) [1].

REFERENCES

1. Štajner, T., Vasiljević, Z., Vujić, D. et al. *J. Clin. Microbiol.* **51**(8), 2686-90 (2013).

Junctions and Contacts in 2D Semiconductor Devices

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Abstract. As 2D materials-based electronics evolve towards very large-scale integrated circuits, one of the major challenges is to achieve high quality contacts with 2D semiconductors. Carrier injection barriers, metal induced gap states and consequently Fermi level pinning at the electrode interfaces hinder the integration of 2D semiconductors. The intrinsic properties of the 2D channel material are seldom accessible, as usually most of the bias for carrier transport is used to overcome the contact-related junctions. Furthermore, in the case of polycrystalline films and assembled nanosheet networks, junctions between adjacent domains and nanosheets also govern the macroscopic response of the devices.

This talk will focus on single crystalline MoS_2, WSe_2, $PtSe_2$, and on liquid phase exfoliated and liquid-liquid interface assembled MoS_2 nanosheet networks. We will review several possible electrode options, from organic self-assembled monolayers functionalized conventional metals [1], to van der Waals semi-metallic contacts [2,3]. The focus will be on ways to evaluate contact-related losses, considering macroscopic electrical measurements, device modeling, and local probing of the electrostatic potential by in-operando Kelvin probe force microscopy [1-4]. We will see how contact engineering can improve the properties of 2D semiconductor devices and also tailor carrier injection into 2D channels.

REFERENCES

1. Matković, A., et al., Interfacial band engineering of MoS_2/gold interfaces using pyrimidine-containing self-assembled monolayers: toward contact-resistance-free bottom-contacts. *Adv. Electron. Mater.* **6**, 2000110, (2020).
2. Murastov, G., et al., Multi-Layer Palladium Diselenide as a Contact Material for Two-Dimensional Tungsten Diselenide Field-Effect Transistors. *Nanomater.* **14**, 481, (2024).
3. Aslam, M.A., et al., All van der Waals Semiconducting $PtSe_2$ Field Effect Transistors with Low Contact Resistance Graphite Electrodes. *Nano Lett.* **24**, 6529, (2024).
4. Gabbett, C., et al., Understanding how junction resistances impact the conduction mechanism in nano-networks. *Nat. Commun.* **15**, 4517, (2024).

Neutrons and Photons Elevating Worldwide Science (NEPHEWS) – Trans-National Access For Excellent Curiosity Driven Research

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Abstract. NEPHEWS – the Neutrons and Photons Elevating Worldwide Science – is an Horizon Europe Co-funded project-based access program targeting new and non-expert users and user communities, driven by the neutron and photon European user communities [1]. It delivers access to the world-class collective of Europe's premiere open advanced neutron, synchrotron and free-electron laser complementary research infrastructures (RI), to promote curiosity driven excellence in research. The bottom-up User-to-User-oriented approach aims to build an integrated European RI landscape involving LEAPS and LENS consortia and their European scientific user communities. New and non-expert users receive in-depth hands-on expert training in twinning research experiments with expert-users, complimented with support in virtual access, workshops, schools and proposal writing. All build expertise, foster collaborations, and widen user access across the European Research Area. NEPHEWS specifically engages user and scientific communities of selected priority countries – of which **Serbia** is one – via outreach visits, priority access, and supporting political dialogue of national user communities with national funding authorities. The simultaneous effort for neutrons, free electron lasers and synchrotrons across Europe reduces the access barrier for using these techniques, sustains the user communities and helps to provide knowledge transfer between the user communities, to industry and the wider society researchers of neutron and photon sources worldwide is provided. Specific reference and statistics of the participation by Serbian researchers in worldwide neutron and photon facilities will be highlighted [2] along with opportunities for participation in NEPHEWS programmes.

REFERENCES

1. NEPHEWS project webpage, https://beamtime.eu/
2. Stankovski, M and Khotbehsara, F. A. P, "What is the size of the global light- and neutron source research communities?", Lund Institute of Advanced Neutron and X-ray Science, May 2024, https://www.linxs.se/news/article-series-i/size-of-the-global-light-and-neutron-source-communities

Observing On-Surface Synthesis of Novel Nanostructures By High Resolution Synchrotron Based X-ray Spectroscopies: Chiral Graphene Nanoribbons and Porphyrin Networks

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Abstract. On-surface synthesis (OSS) has rapidly grown since the seminal synthesis of atomically precise armchair edge graphene nanoribbons or 7-AGNR arising from halogenated molecular precursors such as 10,10´-dibromo-9,9´-bianthracene (DBBA). [1] The diversity of possible GNR, their morphologies, the heteroatom internal or edge doping, the formation of heterostructures, or employing differing hierarchical nanostructure synthesis as was demonstrated with bi-halogenated porphyrins [2] has resulted in an explosion of investigations. The playground of OSS begins with gold growth surfaces (though not limited to these); relies on thermally assisted dehalogenation of precursors and their on surface-assisted Ullmann coupling; finally exploiting higher temperature cyclodehydrogenation (CDH) giving planarization of these nanostructures. Primary investigations typically employ STM and/or bond-resolved AFM, but synchrotron radiation-based x-ray spectroscopy give additional insights into these materials. An overview of our recent work will focus on ultra-high resolution core level C 1s, and N 1s XPS and C, B, O, and N K-edge NEXAFS in i) heteroatom edge doped (4,1)-chiral GNR embedding oxygen-boron-oxygen motifs on the zigzag edges [3] on Au(788) and Ag(111) surfaces and ii) aligned one-dimensional CDH-porphyrin chains on Au (788) surfaces arising from Nickel:5,15-dibromophenyl,15,20-diphenylporphyrin precursors. In each case distinct spectroscopic changes occur during the three stages of OSS. Further, for the planarized π- conjugated 1D CDH nickel-porphyrin chains, the final C 1s XPS of the linked extended-porphyrin moieties exhibits shake-up features at lower energies from the main photoelectron lines. All spectra are simulated through density functional theory (DFT) using the StoBe implementation [4].

REFERENCES

1. Cai, J. et al., Nature 466, 470–3 (2010).
2. Lafferentz, L., et al. (2012). *Nature Chemistry*, *4*(3), 215–220.
3. Wang, X.-Y. et al., J. Am. Chem. Soc. 140, 9104–9107 (2018).
4. Hermann, K., Pettersson, L.G.M et al., StoBe-deMon v3.3 (2014). https://www.fhi.mpg.de/1022673/StoBe

Strongly Anisotropic Spinterface Magnetism in Cobalt/Molecular Heterostructures

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Abstract. We investigated influence of metal/organic-molecules interfaces on the magnetic dynamics in thin polycrystalline Co thin films by means of the time resolved coherent spin wave (CSW) spectroscopy [1]. We compare the effects of interfacing the Co films to a nonmagnetic metal (Al), tris(8-ydroxyquinoline)gallium (Gaq_3), M-phthalocyanines (M=Cu, Co) and Buckminster-fullerene (C_{60}) molecules. The thin Co films interfaced with molecular layers display strong hardening of the CSW frequency at low *T* with a transition in the 170 K - 200 K range. The behavior is found to be very similar for different molecular species/shapes and can be attributed to the presence of a strongly-anisotropic magnetic ordering at the hybridized interface (spinterface) that is not directly related to the bulk Co-film magnetism and sets in below T~170 K.

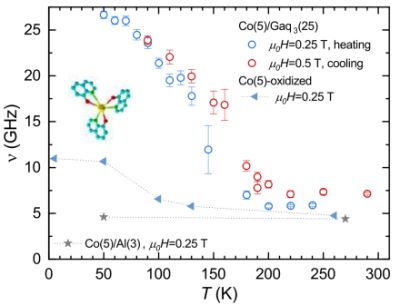

FIGURE 1. The spin-wave frequency as a function of temperature at a constant external magnetic field in the Co(5 nm)Gaq_3(25 nm) sample compared to the reference Co(5 nm)/Al(3 nm) sample and oxidized Co(5 nm) film.

REFERENCES

1. M. van Kampen et al., Phys. Rev. Lett. 88 227201 (2002).
2. T. Moorsom et al., Phys. Rev. B. 101 060408 (2020).

Allergies of the Respiratory Tract: Fungi as the Neglected Allergens

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Abstract. Fungal allergens are increasingly recognized as significant contributors to respiratory tract (RT) allergic diseases, yet they remain largely overlooked in clinical practice. Over 30% of the global population suffers from at least one allergic disease, and today this number exceeds 40% in Europe [1]. Among the spectrum of allergic fungal airways disease (AFAD), fungi can cause or exacerbate conditions such as allergic fungal rhinosinusitis (AFRS), allergic bronchopulmonary aspergillosis/mycosis (ABPA/M), and severe asthma with fungal sensitization (SAFS). Thermotolerant molds like *Aspergillus fumigatus*, *Bipolaris* spp., and *Curvularia* spp. are most frequently implicated, alongside non-thermotolerant genera such as *Alternaria* and *Cladosporium* [2]. Fungal allergens such as proteases (e.g., Asp f13) disrupt epithelial integrity and trigger type I hypersensitivity reactions, with eosinophilic inflammation, mucus overproduction, and bronchiectasis as hallmark features. However, the diagnosis remains challenging due to variability in fungal extract composition and limitations in skin and serologic testing [3]. The lack of standardized fungal allergen panels further complicates immunotherapy development.

Effective control strategies include allergen avoidance, air purification, antifungal treatment (e.g., itraconazole), asthma management, surgical intervention in AFRS, and potential immunotherapy. Despite their ubiquity and significant clinical impact, fungal allergens are insufficiently addressed in current guidelines, warranting greater awareness and targeted research.

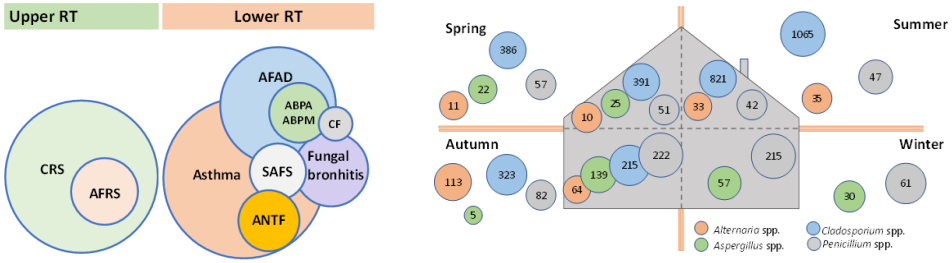

FIGURE 1. Allergic fungal airways disease conditions (left) and mean concentrations (m^3) of fungal spores in indoor and outdoor environments associated with AFAD (right).

REFERENCES

1. European Federation of Allergy and Airways Diseases Patients Associations. https://www.efanet.org/inform/patient-evidence/allergy
2. Wardlaw, A. J., Rick, E. M., Pur Ozyigit, L., Scadding, A., Gaillard, E. A., & Pashley, C. H. New Perspectives in the Diagnosis and Management of Allergic Fungal Airway Disease. *Journal of asthma and allergy*, ***14***, 557-573 (2021).
3. Pfeiffer, S., & Swoboda, I. Problems Encountered Using Fungal Extracts as Test Solutions for Fungal Allergy Diagnosis. *Journal of fungi (Basel)*, ***9***, 957 (2023).

Anisotropic Strain Response in FeSe

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Abstract.

Unconventional superconductivity often arises in materials with complex interactions, where competing ordered states such as magnetism, nematicity, and superconductivity, interact and sometimes overlap, making their nature elusive. Among iron-based superconductors, the isostructural FeSe and FeS may appear similar but they differ significantly in their physical properties. While FeSe undergoes a nematic and structural phase transition, FeS shows no structural transition even at the lowest temperatures, with its critical temperature (T_c) halved compared to FeSe. Interestingly, substituting selenium with sulfur in FeSe suppresses the nematic transition temperature to zero near a quantum critical point (QCP), which coincides with a significant drop in T_c. It has been suggested that while spin-fluctuations dominate below the QCP and significantly affect electron-phonon interactions, nematic fluctuations become prominent above the QCP. Here, we present a detailed Raman scattering study of FeSe under uniaxial strain applied along two high-symmetry crystallographic directions, ⟨110⟩ and ⟨100⟩, to investigate how symmetry-breaking perturbations affect its lattice dynamics. Our results reveal a pronounced anisotropy in the phonon response to strain: orthorhombic distortion along the ⟨110⟩ direction leads to a moderate narrowing of the temperature window over which phonon anomalies occur, while strain along ⟨100⟩ which introduces rhombohedral distortion, results in a significant broadening of the temperature range over which phonon mode splitting, and energy and linewidth anomalies are observed. We find that the fully symmetric A_{1g} phonon mode is particularly sensitive to symmetry-breaking perturbations, while the B_{1g} phonon mode remains largely unaffected.

*This research was supported by the Science Fund of the Republic of Serbia, 10925, Dynamics of CDW transition in strained quasi-1D systems - DYNAMIQS

Tuning the Properties of Liquid-Phase Exfoliated Langmuir-Blodgett Assembled Graphene Films via Chemical Doping

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Abstract. The increasing interest in graphene and other 2D materials extends across scientific and technological fields, shifting from fundamental research to practical applications. Doping plays a crucial role in tailoring their electrical, optical, and magnetic properties, broadening their usability. Among various scalable synthesis methods, liquid-phase exfoliation (LPE) followed by Langmuir-Blodgett (LB) deposition enables the fabrication of thin graphene films with excellent substrate coverage, offering high reactivity and tunability. Chemical doping with nitric acid for p-doping significantly enhances the sheet conductivity (five times) of LPE LB graphene films, improving their potential for electronic applications [1]. Furthermore, we developed a single-step doping strategy, replacing water with metal standard solutions as the liquid subphase, that integrates film formation and doping at the liquid-air interface [2]. By employing Li-based salts for n-doping and Au-based salts for p-doping, we achieved a tunable work function spanning nearly 1 eV, making these films suitable for electron and hole injection interfaces in optoelectronics. Beyond electronic modifications, we used the single-step approach to introduce localized magnetic domains into nonmagnetic LPE LB films via Fe nanoparticle functionalization, exploring their potential for heavy metal water purification. Raman and XPS confirmed successful surface modification, while MFM revealed a strong phase shift (~0.2°), indicating localized magnetic moments absent in unmodified films.

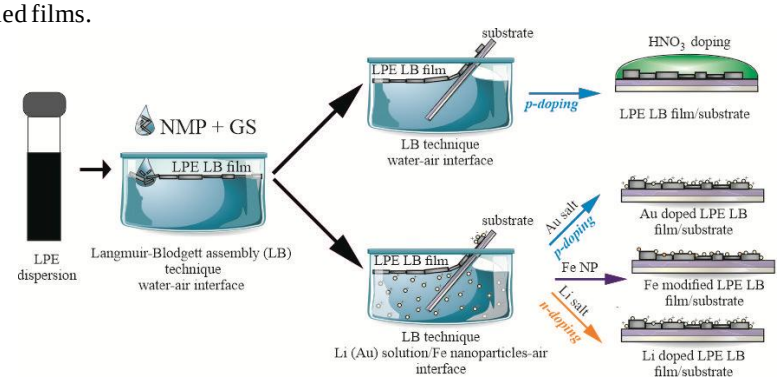

FIGURE 1. Fabrication and chemical doping of Liquid-Phase Exfoliated Langmuir-Blodgett Assembled Graphene Films (LPE LB) Graphene Films.

REFERENCES

1. Matković A. et al., *2D Mater.* **3**, 015002 (2016).
2. Milošević I. R. et al., *Sci. Rep.* **10**, 8476 (2020).

Brain-inspired computing with superconducting neurons

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Abstract. While modern experimental techniques are enabling increasingly multifold studies of superconductivity (from in-situ synthesis to transport and scanning-probe measurements), the community has witnessed an increasing gap between the ab initio calculations and those on mean-field levels, and even more to the desired device modelling. At present, the only tool able to address the needed multi-scale modelling of superconductors, nanopatterned into electronic circuitry, are the advanced Ginzburg-Landau simulations. Over the years we have developed a multiscale approach where information about fermiology, vibrational modes, and electron-phonon coupling are obtained from first principles for the materials of interest, to be subsequently translated into (anisotropic) superconducting properties, that can further serve to properly parameterize mean-field models in order to capture the behavior of that superconductor when nanoengineered into an electronic device [1-4].

In this talk, I will review our most recent breakthroughs in that respect, and show particular numerical design of superconducting circuitry (on advanced size and time scale), with focus on the realizations of superconducting artificial neurons [5] and field-effect transistors [6], as the key elements for scalable yet energy-efficient computational architectures of the future.

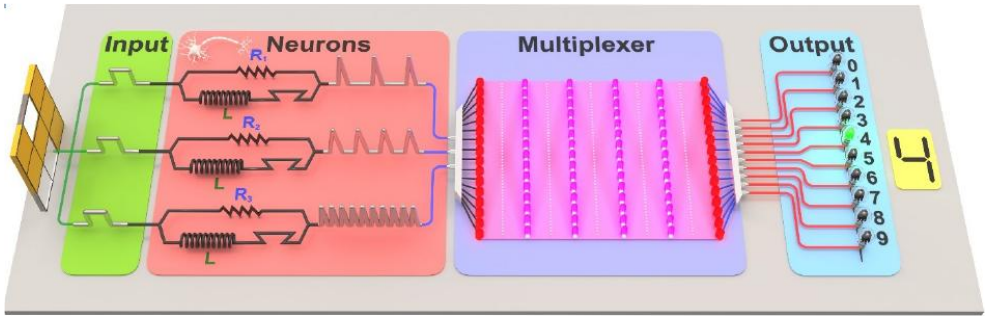

FIGURE 1. The neuromorphic circuit of shunted superconducting nanowires, for image or voice recognition.

REFERENCES

1. L. Embon et al., Nature Commun. 8, 85 (2017).
2. J. Lombardo et al., Nanoscale 10, 1987 (2018).
3. R. Cordoba et al., Sci. Rep. 9, 12386 (2019).
4. Y.-Y. Lyu et al., Nature Commun. 12, 2703 (2021).
5. E. Toomey et al., Nano Lett. 20, 8059 (2020).
6. G. De Simoni et al., Nature Nanotechnology 13, 802 (2018); M. F. Ritter et al. Nature Electronics 5, 71 (2022).

Invisible Defense With Luminescent Polish For Anti – Counterfeiting

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Abstract. We develop an innovative and simple luminescent polish which would serve as a concealed yet easily detectable marker for authenticity verification. Our product strives to be meticulously engineered to excel in two critical aspects: cost – effective manufacturing and uncompromising quality which could potentially outshine the competition in today's crowded market. We use well established classical ceramic method for synthesis of europium – doped yttrium vanadium oxide nanopowders (YVO_4: Eu^{3+}).YVO_4: Eu^{3+} is a well known red ceramic phosphor. YVO_4 is chosen since it is an attractive host material for rare earth ions that could be well excited under UV light irradiation. By incorporating these nanoparticles into polish formulations we create a unique anti – counterfeiting solution: a luminescent coat for objects or documents, detectable under UV light, providing a reliable method for authentication. This has many advantages compared to traditional anti – counterfeiting strategies, such as barcodes, watermarks or micro printing, which are easily copied and difficult to effectively prevent counterfeiting. While luminescent ink has played a crucial role in authentication over the years, its complex application processes and limited versatility have become apparent drawbacks. The need for specialized printing equipment and trained personnel has led to increased production costs and logistical challenges. In stark contrast, luminescent polish can be effortlessly applied to a wide range of surfaces using conventional methods, making it accessible and cost – effective. Furthermore, luminescent polish offers a unique advantage in terms of visibility and durability. Its luminescent patterns are easily discernible under UV light, enabling quick and reliable authentication. Unlike luminescent ink, which can fade over time or be susceptible to wear and tear, luminescent polish adheres more robustly to surfaces, ensuring long – lasting security features.

A Simple and Practical Approach for Calculating Transport Properties with Dynamical Quantum Typicality: Application to the Holstein Model

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Abstract. Although important for practical applications, the accurate theoretical calculation of transport properties is a notoriously hard problem. The challenge stems from the exponential growth of the Hilbert space with system size. This difficulty can be leveraged to our advantage by using the insight that even a single, randomly chosen pure state in a high-dimensional Hilbert space can effectively represent the entire statistical ensemble [1]. This greatly simplifies the computation of the current-current correlation function, which, within linear response theory, directly determines the frequency-dependent mobility. The time evolution of the current-current correlation function is handled using the Runge-Kutta scheme. As a result, we achieve a simple, transparent method that is easy to implement, with computer memory requirements and computational effort scaling linearly with the Hilbert space dimension and the time grid length. Although this approach can be applied to a wide range of systems, we restrict our numerical results [2] to the Holstein model, for which several reliable benchmarks are available [3]. We demonstrate that QT effectively complements other currently employed methods by overcoming some of their inherent limitations.

REFERENCES

1. Heitmann, T., Richter, J., Schubert, D., and Steinigeweg, R., *Z. Naturforsch. A* **75**, 421 (2020).
2. Mitrić, P., arXiv:2412.17436 [cond-mat.str-el] (under review in Phys. Rev. B).
3. Janković, V., *J. Chem. Phys.* **159**, 094113 (2023).

Kagome Thin Layers: Diperiodical Point of View

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Abstract. Layered kagome materials have arisen as a fertile platform for exploring connection of frustrated geometry and various interesting physical properties. Producing thin kagome layers reveals importance of using their exact symmetry, layer groups. Here, overview of hypothetical diperiodic structures containing exact kagome lattice, including possible magnetic ordering is given. Detailed symmetry based analysis, including deformations controlled by symmetry, is good starting point for thorough research of influence of symmetry on various physical phenomena.

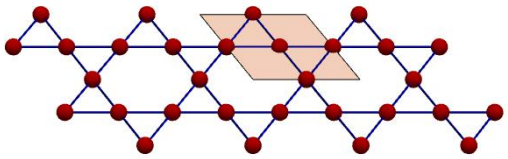

FIGURE 1. Monoatomic Kagome layer

REFERENCES

1. Kim, S. W., Oh, H., Moon, E. G. et al., *Nature Communications*, **14**, 591 (2023).
2. Milošević, I., Nikolić, B., Damnjanović, M., and Krčmar, M., *J. Phys. A* **31**, 3625-48 (1998).
3. Kopsky, V. and Litvin, D. B., *International Tables for Crystallography, Volume E, Subperiodic groups*, International Union of Crystallography, Dordrecht/Boston/London: Kluwer Academic Publishers, 2002.
4. Litvin, D. B., *Magnetic Group Tables*, International Union of Crystallography, 2013.
5. Nikolić B., Milošević, I., Vuković, T., Lazić, N., Dmitrović, S., Popović, Z. P. and Damnjanović, M., *Acta Crystallographica Section A* **78**, 107-114 (2022).

How Ultrafast Demagnetization Drives Spin and Charge Currents and the Ensuing THz Radiation

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Abstract. The ultrafast demagnetization is a surprising phenomenon discovered in 1996 in which a femtosecond laser pulse irradiating a ferromagnetic metallic layer leads to its magnetization vector shrinking in length while not rotating. Despite being one of the primary experimental observables, THz electromagnetic radiation from either a single magnetic layer, or much more enhanced from ferromagnet/spin-orbit-material bilayers, has rarely been rigorously calculated. This has forced experimentalists to rely on qualitative pictures of how spin currents are generated and converted into charge currents in systems exhibiting ultrafast demagnetization. This talk will discuss very recently developed framework [1], combining time-dependent density functional theory and Jefimenko formulas for time-retarded electric and magnetic fields as proper solutions of the Maxwell equations, which makes it possible to compute emitted THz radiation from a microscopic and first-principles viewpoint. Inspection of currents as sources of the electric field in the far-field region within Jefimenko formulas then reveals that a major contribution to THz radiation arises from completely overlooked charge current within the ferromagnetic layer that is pumped by demagnetization dynamics. Spin current is also pumped by demagnetization dynamics, and it flows toward spin-orbit-material layer where it is converted into charge current as often assumed. Its origin can be accounted by the same time-dependent quantum transport calculations [2] which explain spin pumping by rotating magnetization of fixed length when ferromagnets are driven by microwave photons of much lower energy than in ultrafast demagnetization phenomena. However, due to multiple spin-to-charge conversion processes, connection between pumped spin current and charge current within spin-orbit-material is not straightforward, as also observed experimentally, while thus converted charge current is not necessarily a major contributor to THz radiation as often assumed in qualitative pictures.

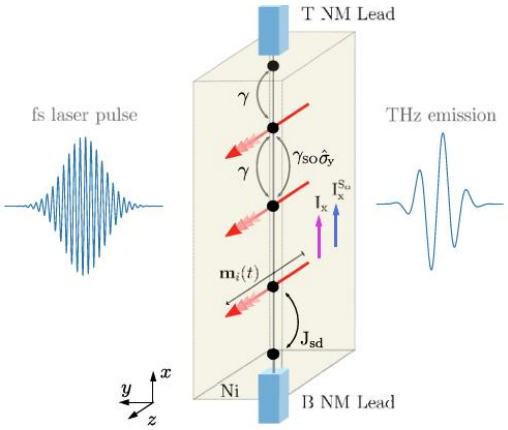

FIGURE 1. Illustration of femtosecond laser pulse which leads to shrinking of local magnetization (red) vectors of ferromagnetic metallic layer (such as Fe, Co, Ni). In turn, such demagnetization dynamics introduces time-dependent driven into the sea of electrons, thereby pumping their charge current that radiates electromagnetic waves at THz frequencies.

REFERENCES

1. Kefayati, A., and Nikolić, B. K., *Phys. Rev. Lett.* **133**, 136704 (2024).
2. Varela-Manjarres, J., Kefayati, A., Jungfleisch, M. B., Xiao, J. Q., and Nikolić, B. K., *Phys. Rev. B* **110**, L060410 (2024).

The stress-strain relationship of quantum materials: New method developments and application to Sr_2RuO_4

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Abstract.

Over the past decade, uniaxial pressure has emerged as a powerful tuning method for quantum materials, as it allows for the controlled breaking of lattice symmetries. Driven by technical advances, investigations under uniaxial pressure have extended beyond the study of electronic properties to include the measurement of the crystal's elasticity. A strong entanglement between the electrons and the lattice has been identified across various correlated electron systems. Key examples include the discovery of giant non-linear elasticity linked to nematic order [1] and Mott metal-insulator transitions [2], as well as, more recently, the observation of pronounced lattice softening in the normal state of the unconventional superconductor Sr_2RuO_4 when tuned across an electronic Lifshitz transition by uniaxial pressure [3].

In this talk, I will introduce A.C. stress-strain measurements [4] as a technique for investigating the elastic properties of quantum materials under uniaxial pressure. Using Sr_2RuO_4 as an example, I will show that this method is not only effective for detecting phase transitions but also for probing low-frequency lattice dynamics in their vicinity. At the end of the talk, I will discuss A.C. stress-strain measurements on other quantum materials, highlighting the broad applicability of this approach.

*Work is supported by the DFG through TRR 288–422213477.

REFERENCES

1. Böhmer and Meingast, *C. R. Physique* **17**, 90 - 112 (2016).
2. Gati *et al.*, *Sci. Ad.* **2**, e1601646 (2016).
3. Noad *et al.*, *Science* **382**, 447 (2023).
4. O'Neil *et al.*, *Rev. Sci. Instrum.* **95**, 073909 (2024).

Strain-dependent vibrational properties of $SrIrO_3$ thin films

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Abstract. Ruddlesden-Popper series of 5d strontium-irridates ($Sr_{n+1}Ir_nO_{3n+1}$) have been extensively studied in the past years due to its unique properties, including spin-orbit coupling, crystal field and electronic correlations. Interplay between these features facilitates transitions between different electronic states due to slight structural or chemical changes. In this work Raman spectra of $SrIrO_3$ thin films grown on different substrates (LAO, LSAT, STO, GSO) are investigated for various sample orientations and light polarizations. Our attention is focused on Raman mode appearing around 395 cm^{-1}, which is assigned as A_g symmetry mode by orientation-dependent measurements. A blue shift of this mode when going from SIO/GSO, through SIO/STO and SIO/LSAT, to SIO/LAO sample, was observed, which is a clear fingerprint of increasing compressive strain, induced by substrate.

Magnon Spin Transport in Antiferromagnetic Insulators

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Abstract. Quantized excitations of the spin system in magnetically ordered materials, i.e. magnons, offer a unique platform for future information technology. Magnonic spin transport in combination with the possibility of electrical injection, control, and detection paves the way for the realization of novel spintronic devices [1,2]. Antiferromagnetic materials host pairs of spin-up and spin-down magnons as their quantized spin excitations. We describe them in terms of a magnonic pseudospin [3,4]. Its close analogy to the electronic spin led to the prediction of novel fascinating magnon transport phenomena [3-6]. We here investigate the magnon propagation in the electrically insulating antiferromagnetic oxide α-Fe_2O_3 (hematite). It harbors a finite Dzyaloshinskii-Moriya interaction [7,8] together with an easy-plane anisotropy, resulting in a slight canting of the sublattice magnetizations in the (0001) plane at room temperature and, hence, in a residual net magnetic moment [9]. In this situation, the magnon pseudospin precesses coherently about the equilibrium pseudofield, the latter capturing the nature of the magnonic eigenexcitations in the antiferromagnet [3]. We demonstrate this precession via the magnon Hanle effect [4]. Its realization by electrically injected and detected magnons in an antiferromagnetic insulator promises a high potential for devices [4,5,9,10]. We further observe a nonreciprocity in the magnon Hanle signal, depending on the magnon propagation direction between spin injector and detector electrodes [10]. Interchanging their roles alters the detected magnon spin signal. The recorded difference depends on the applied magnetic field and reverses sign when the signal passes its nominal maximum at the so-called compensation field [10]. We explain these observations in terms of a spin transport direction-dependent pseudofield. The latter leads to a nonreciprocity, which is found to be controllable via the applied magnetic field.

REFERENCES

1. Ludo J. Cornelissen *et al.*, *Nature Physics* **11**, 1022 (2015).
2. Romain Lebrun *et al.*, *Nature* **561**, 222 (2018).
3. Akashdeep Kamra *et al.*, *Physical Review B* **102**, 174445 (2020).
4. Tobias Wimmer *et al.*, *Physical Review Letters* **125**, 247204 (2020).
5. Janine Gückelhorn *et al.*, *Physical Review B* **105**, 094440 (2022).
6. Andrew Ross *et al.*, *Applied Physics Letters* **117**, 242405 (2020).
7. Igor E. Dzyaloshinsky, *Journal of Physics and Chemistry of Solids* **4**, 241 (1958); Journal of Experimental and Theoretical Physics (JETP) **19**, 960 (1964).
8. Tôru Moriya, *Physical Review* **120**, 91 (1960).
9. Monika Scheufele *et al.*, *APL Materials* **11**, 091115 (2023).
10. Janine Gückelhorn *et al.*, *Physical Review Letters* **130**, 216703 (2023).

Graphene-based Composite Thin Films with Self Assembling Biomolecules as Active Elements in Sensors

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Abstract. Each 2D-material thin film can be regarded as a composite of a solid (having a periodic structure within the plane) and a molecule (aligned with the direction perpendicular to its surface), characterized by relatively weak interlayer bonds. Significant structural changes in either a lateral or vertical direction are having a substantial impact on the chemical and physical properties of materials. The performance and precision of electrochemical and biochemical sensors based on graphene heavily depend on how effectively the process of interest is integrated with its properties and the environmental conditions, particularly ambient humidity. Notably, the sensitivity of 2D-materials to environmental conditions has been beneficial for use in sensing devices, especially for detecting pollutants in air and water [1-3]. Consequently, it is essential that these sensors operate with accuracy and dependability in ambient conditions where air moisture significantly contributes to channel material degradation and conductivity reduction. Functionalizing graphene with biomolecules has been shown to be a highly effective strategy for graphene-based electrical sensors, which can detect proteins, DNA, pesticides, bacteria, antibodies, and heavy metals in water and air due to their high binding affinity to inorganic contaminants [4]. For these applications, understanding how humidity and water from the analyte solutions affect the composition and surface properties of these heterostructures is necessary. In our work, we analyzed the combination of a nucleic base thymine (Thy) and two types of lipid molecules (dipalmitoyl-phosphatidyl-choline - DPPC, Sphingomyelin) on top of the graphene films formed by the transfer of graphene nanoflakes from liquid-phase exfoliation. The distribution and molecular arrangement of thymine and lipid molecules on the surface differ depending on the structure and water-repelling properties of the graphene film. To understand how water in the surrounding environment affects the adsorption of thymine and lipids onto graphene films, we conducted Near-Ambient X-ray Photoelectron Spectroscopy experiments. These experiments involved exposing pure graphene and graphene-based composites to 1 and 5 millibars of pure gaseous water within an ultra-high vacuum reaction chamber at room temperature. Additionally, the UV-Vis and Raman vibrational spectra of composite thin films were examined, and atomic force microscopy was employed to study their surface characteristics. The findings from these experiments are analyzed with consideration for the operation of these heterostructures as active components in field-effect transistor chemical sensors.

REFERENCES

1. Anichini, C., Czepa, W., Pakulski, D., Aliprandi, A., Ciesielski, A., and Samorı, P., *Chem, Soc, Rev*, **47**, 4860 (2018)
2. Perreault, F., Fonseca de Fari, A., and Elimelech, M., *Chem. Soc. Rev*., **44**, 5861 (2015)
3. Li, P., Liu, B., Zhang, D., Sun, Y., and Liu,J., *Appl. Phys. Lett*. **109**, 153101 (2016)
4. Mao, S., Chang, J., Pu, H., Lu, G., He, Q., Zhang, H., and Chen, J., *Chem. Soc. Rev*., **46**, 687 (2017)

Crystal Structure Predictions in Correlated Materials at Finite Temperatures

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Abstract. Solving crystal structures from scattering experiments can sometimes be challenging due to the lack of single-crystal samples or the complexity of the crystallographic model. In this talk, we will discuss the numerical methods used to predict crystal structures and explore their advantages and disadvantages. We will demonstrate these through a series of compounds in the paramagnetic insulating, metallic, and metallic-to-insulating transition states [1,2]. We will argue that density functional theory, combined with embedded dynamical mean field theory as implemented in the eDMFT code [3], can be used to understand and quantitatively predict the electronic-structural interplay in complex correlated materials at finite temperatures.

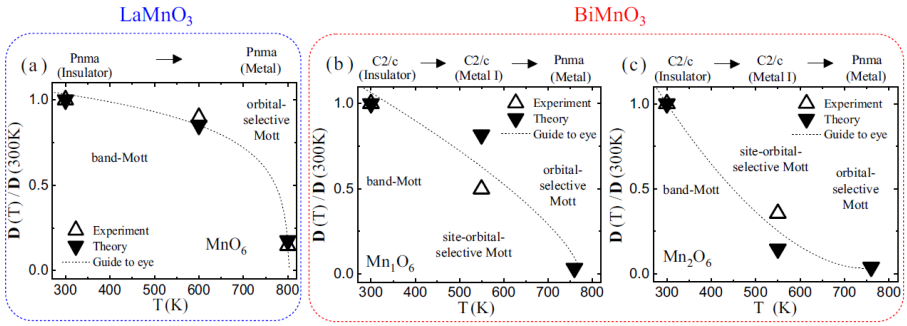

FIGURE 1. Structural relaxations within LDA + eDMFT for all the temperature-dependent novel electronic phases in (Bi,La)MnO_3. In each panel we plot the bond distortion (D) index versus temperature, normalized to its values at room temperature. In panel (a) we plot D for the Mn site in $LaMnO_3$. In panels (b) and (c) we plot D for the two inequivalent Mn sites in $BiMnO_3$. Above each panel we give the temperature dependent crystal symmetry and the properties of that electronic state (metal or insulator). The arrows point to the type of phase transition (structural or metal-insulator phase transition).

Part of this work was supported by a grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2019-1767, within PNCDI III.

REFERENCES

1. K. Haule, G. L. Pascut, Scientific Reports 2017, 7, 10375.
2. G. L. Pascut, K. Haule, Phys. Rev. B 2023, 107, 045147.
3. http://hauleweb.rutgers.edu/tutorials/Overview.html

Unraveling the Electrochromic Mechanism of Ni-Deficient NiO: A Charge Localization Perspective from DFT+*U* Calculations

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Abstract. A crucial aspect of sustainable energy systems is improving energy efficiency, particularly in heating and cooling for residential and commercial buildings. Electrochromic (EC) materials have emerged as promising candidates for smart windows and energy-saving applications due to their ability to reversibly switch between transparent and colored states under an applied voltage [1]. Among various EC materials, nickel oxide (NiO) is one of the most widely studied, yet its electrochromic mechanism remains a topic of debate, especially in Li^+-containing electrolytes. In this work, we employed DFT+*U* calculations to investigate the electrochromism of Ni-deficient NiO, revealing a new mechanism distinct from the conventional view that attributes optical changes solely to variations in Ni^{2+}/Ni^{3+} oxidation states. Our results indicate that in bulk Ni-deficient NiO, hole bipolarons form, and ($Li^+ + e^-$) insertion fills one hole state, leaving a single hole polaron in the system. This alteration in the electronic structure directly affects optical properties, leading to a decrease in the absorption coefficient. Interestingly, we observed minimal changes in Ni oxidation states during ($Li^+ + e^-$) insertion. This suggests a general process where hole bipolaron states are filled by adding an electron, largely independent of the specific counterion. Further investigations on Ni-deficient NiO(001) surface with Li^+, Na^+, and K^+ ($+ e^-$) insertion support the broader applicability of this mechanism, providing insights into NiO electrochromism in diverse electrolytes and doped NiO-based materials [2]. These findings offer a new perspective on electrochromic behavior, with implications for the design of advanced EC materials with enhanced performance and stability.

REFERENCES

1. Yang, P., Sun, P., and Mai, W., *Mater. Today* **19**, 394–402 (2016).
2. Pašti, I.A, Dobrota, A.S., Migas, D.B., Johansson, B., Skorodumova, N.V., *Phys. Chem. Chem. Phys.* **25** 7974-7985 (2023).

Modeling and Mapping Current Flow in MoS_2 Nanonetworks

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Abstract. Understanding charge transport in two-dimensional material networks is essential for advancing next-generation electronic devices. In this lecture, we explore the electrical behavior of MoS_2 nanonetworks, focusing on how current paths form and distribute across these complex systems. We present an integrated approach combining nanoscale electrical mapping with diagram-based modeling to understand the interplay between nanosheet morphology, network connectivity, and electrical performance. Using in-operando nanoscale potential measurements, we visualize local potential drops with nanometer resolution, identifying the relative contributions of individual nanosheets and their interconnections. We then introduce a probabilistic, diagram-based model that captures the geometry and connectivity of the MoS_2 network, enabling the simulation of current flow and the prediction of dominant conduction paths. This modeling framework allows us to link microscopic features to macroscopic device performance, providing insights into how material quality, connectivity, and network density impact overall transport. Finally, we connect these findings to electrical measurements using the Y-function approach, offering a robust method to quantify non-field-modulating resistance elements in the network. Together, these methods provide a comprehensive picture of current flow in MoS_2 nanonetworks and highlight pathways for optimizing material processing and device architecture for improved electronic performance.

REFERENCES

1. Jelena Pešić, Simon Leitner, Joseph Neilson, Igor Stanković, Muhammad Zubair Khan, Dragana Tizić Matković, Adam G. Kelly, Tian Carey, Jonathan Coleman, Aleksandar Matković. Imaging Junctions in Two-Dimensional Semiconductor Nanosheet Network Transistors, under review.

Fermi Surface Characteristics in FeP_2

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Abstract. Marcasite compounds show an interesting interplay of spin, orbital, and lattice degrees of freedom and host properties relevant for applications and fundamental science. Electronic correlations that arise in this context are critical for tuning conductivity which is of interest in electrochemical reactions in catalysis but are also important to understand high values of cryogenic thermoelectric power factor in materials with 3*d* orbitals related to classical rare earth Kondo semiconductors. FeP_2 marcasite is isostructural to small gap Kondo-insulator-like semiconductor $FeSb_2$. It exhibits a cascade of temperature-induced spin but also conducting state transitions as temperature is lowered from the room-temperature high spin (HS) state [1]. There is metal-to-semiconductor transition on cooling to intermediate spin (IS) state below 120 K and semiconductor-to-bad-metal transition below 20 K as FeP_2 enters low spin (LS) state. In my talk I will present Fermi surface characteristics of the bad metal [2]. Quantum oscillations are composed of three main oscillation frequencies with rather light carrier mass, about few tenths of bare electron mass on some pockets. Despite three-dimensional character of the unit cell and the absence of the van der Waals bonds, angular-dependence of observed frequencies indicates the presence of a two-dimensional Fermi surface sheet with trivial Berry phase but also two three-dimensional Fermi surface sheets with possible non-trivial Berry phase.

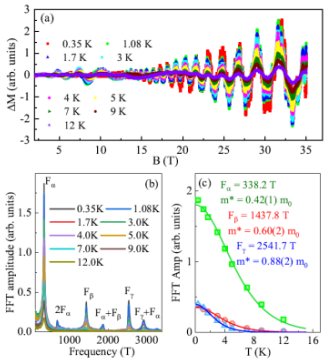

FIGURE 1. Bacground-subtracted temperature dependent dHvA signal in FeP_2 (a) showing clear oscillations. The FFT of the subtracted data (b). Lifshitz-Kosevich fit of the dHvA amplitude (c).

REFERENCES

1. Du, Qianheng et al., *Chem. Mater*. **34**, 2025 (2022).
2. Du, Qianheng et al., *Submitted* (2025).

The Role of Metallic Substrates in Large-Area Exfoliation of TMDCs

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Abstract. Gold-assisted exfoliation has emerged as an effective technique for selectively obtaining large-area monolayers of transition metal dichalcogenides (TMDCs), yet its underlying mechanism is still a subject of debate [1,2]. While other metals can also facilitate exfoliation, their practical use is limited by oxidation of their surface [3].
In this study, we systematically investigate six MoS_2/metal heterostructures prepared via direct mechanical exfoliation onto metallic surfaces under controlled atmosphere conditions (Fig. 1a-f). Our results obtained through ultraviolet photoelectron spectroscopy, X-ray photoelectron spectroscopy, and Raman spectroscopy (Fig. 1g) reveal significant variations in interfacial interactions depending on the choice of the metal. Density functional theory calculations further corroborate the variation in the interaction. These results reveal the impact of metal substrates on the electronic structure and vibrational properties of MoS_2. Furthermore, our findings provide fundamental insights into the mechanisms driving metal-assisted exfoliation.

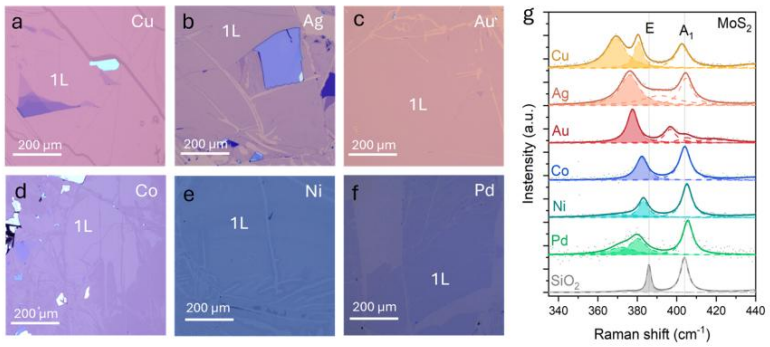

FIGURE 1. (a-f) Optical images of large-area MoS_2 monolayers exfoliated on Cu, Ag, Au, Co, Ni, and Pd. (g) Raman spectra of MoS_2 monolayers exfoliated on different metals.

REFERENCES

1. Velický, Matej, et al., ACS nano, **12.10**, 10463-10472 (2018)
2. Ziewer, Jakob, et al., Advanced Materials, 2419184 (2024)
3. Velický, Matěj, et al., Advanced Materials Interfaces, **7.23**, 2001324 (2020)

Exploring quantum complexity in artificially twisted superconducting heterostructures

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Abstract. Superconductivity is a quantum phenomenon in which certain materials can conduct electricity without resistance below a critical temperature. While the well-established Bardeen-Cooper-Schrieffer (BCS) theory explains this behavior in conventional superconductors at extremely low temperatures, it does not fully capture the complexities of high-temperature superconductors. These materials, often ceramics like cuprates, exhibit superconductivity at temperatures closer to that of liquid nitrogen, making them of great scientific and technological interest. Unlike conventional superconductors, high-temperature superconductors display a complex electronic landscape, where quantum entanglement plays a crucial role. The nature of their superconducting state is not fully understood, and it differs significantly from the classical solid-state physics models found in textbooks. Some researchers refer to these materials as examples of "supreme quantum matter" or "ultra-quantum matter" to emphasize their intricate and unconventional properties. Over the past few decades, advancements in material science have provided a clearer understanding of both the challenges and the potential of these superconductors. A particularly exciting avenue of research involves engineering artificial superconducting structures by stacking and twisting thin layers of cuprates. These heterostructures open the door to novel quantum phases and emergent electronic states that are not found in naturally occurring materials. In this context, ongoing experimental efforts focus on designing and fabricating such systems, addressing technical challenges, and exploring their possible applications in future quantum technologies.

Spin Conduction in FM/AFM/NM Multilayers

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Abstract. Spintronics based on antiferromagnetic materials (AFM) has emerged as a promising candidate for future energy-efficient and high-speed information storage and processing [1]. AFMs offer several advantages over ferromagnets, including higher packing density due to the absence of stray fields and enhanced robustness against external perturbations owing to negligible dipolar fields. Significant efforts have been made to optimize impedance matching and spin-orbit coupling in ferromagnetic/non-magnetic (FM/NM) heterostructures by incorporating an insulating AFM layer. Additionally, long-distance spin information propagation has been attributed to magnon-mediated spin currents. However, the mechanisms governing spin transport in AFMs and their efficiency remain debated. In this work, we review our recent findings on spin conduction mechanisms in FM/AFM/NM heterostructures [2]. Pure spin currents will be injected by spin pumping from a resonant ferromagnet and we will analyze the Inverse Spin Hall Effect measured at the NM layer as a function of the thickness of the AFM layer. The influence of interfacial effects and structural symmetry in the transport of spin currents through the heterostructure will be discussed.

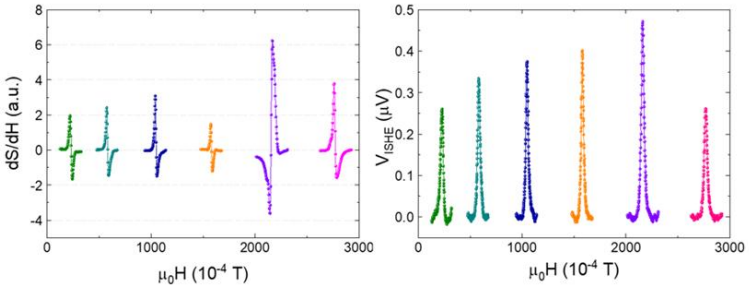

FIGURE 1. Ferromagnetic resonance (left) and Inverse Spin Hall Effect Voltage (right) in a FM/AFM/NM heterostructure at 300K. Measured frequencies are 3, 5, 7, 9, 11 and 13 GHz.

REFERENCES

1. See, e.g., Baltz, V. et al., Rev. Mod. Phys. **90**, 015005 (2018).
2. Chen, S. et al., J. Alloys Comp. **1010**, 177453 (2025). Brown, M. P., and Austin, K., *Appl. Phys. Lett.* **65**, 2503-2504 (1994).

Failed Superconductivity In Chemically Substituted Mott Spin Liquid Materials

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Abstract. A central challenge for understanding unconventional superconductivity in most strongly correlated electronic materials is their complicated band structure and presence of competing orders. In contrast, quasi-two-dimensional organic spin liquids are single-band systems with superconductivity arising near the bandwidth-tuned Mott metal-insulator transition in the absence of other orders. We study chemically substituted κ-organics in which superconducting fluctuations emerge in the phase coexistence region between the Mott insulator and the Fermi liquid. Using magneto-transport and ac susceptibility measurements, we find that global superconductivity fails to set in as temperature $T \to 0$. Our results indicate instead the presence of superconducting domains embedded in the metallic percolating cluster that undergo a magnetic field-tuned quantum superconductor to metal transition. Surprisingly, albeit consistent with the small volume fraction of the metallic percolating cluster, universal conductance fluctuations are seen at high fields in macroscopic samples. The observed interplay of the intrinsic inhomogeneity and quantum phase fluctuations provides a new insight into failed superconductivity, a phenomenon seen in various materials including other unconventional superconductors, such as cuprates.

Anisotropic Superconductor In Josephson Junction With Rashba Spin Orbit Coupling And Exchange Field

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Abstract. We study Josephson effect in a junction with arbitrarily oriented d-wave superconducting electrodes connected through two ferromagnets with noncolinear magnetizations and insulating interfaces. We solve the scattering problem based on the Bogoliubov-de Gennes formalism, extended to the case of anisotropic superconductors and presence of spin flip scattering due to ferromagnet interlayer. We investigate mutual influence of crystal orientation of superconducting electrodes and angle between magnetizations in ferromagnetic bilayer by calculating critical value of Josephson current, and discuss the possibility to achieve coexistence of three stable states 0, π and $\pi/2$ by varying the angle between magnetizations [1]. By adding Rashba spin orbit coupling at the interfaces of d-wave superconductor and ferromagnets the current-phase relation may exhibit a series of novel features and can change significantly as some relevant parameters are tuned. Since in this kind of junction both time-reversal and space inversion symmetry can be broken, Josephson junction can exhibit supercurrent diode effect characterized by nonreciprocal behavior in the critical supercurrent in two opposite directions, as well as anomalous Josephson current at zero phase bias and magnetoanisotropies of Josephson current. We have shown that diode effect occurs in junction with nonsymmetrical oriented d-wave superconducting electrodes, and that large diode effect can be reached by tuning the crystal axes orientation of d-wave superconductors and optimizing some relevant parameters of the junction. We predict that modulating the strength of the Rashba field or exchange field may induce phase transition which for a certain choice of parameters can be continuous between 0-like and π-like, because different individual transport channels have different phase shifts. The temperature induced phase shift and diode characteristic are investigated as well.

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REFERENCES

1. S. Djurdjević and Z. Popović, Prog. Theor. Exp. Phys. **2021** 083I02 (2021).

Phase Separation in Lightly Doped $La_{2-x}Sr_xCuO_4$ Studied by Cu NMR

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Abstract. Electronic and structural inhomogeneities have been found to be ubiquitous in cuprates, and various forms of nanoscale electronic correlated states have been proposed to arise upon the suppression of long-range AFM order. In lightly doped cuprates substantial electronic inhomogeneity and distinct local environments can form, with the possible appearance of insulating and metallic regions. NMR is a local real-space probe that reflects the range and distribution of magnetic fields and electric field gradients in a sample, and therefore suitable for investigation of local spin fluctuations and microscopic structures. Cu NMR measurements with short spin echo times [1] enable us to systematically study the local properties of the electronic spin system in the region of the phase diagram where the material evolves from the insulating AFM phase to the superconducting state. Single crystals of $La_{2-x}Sr_xCuO_4$ with x between 2% and 8% have been studied [2]. Qualitative changes occur as the Sr concentration increases through x = 5%, which we interpret as signatures of a transition from a state with disconnected metallic islands to a granular metal with tunneling between the grains (Figure 1). Hence, we demonstrate that complex nanoscale electronic phase separation is ubiquitous in LSCO, and that a connectivity transition occurs around the doping level where superconductivity first appears in the phase diagram.

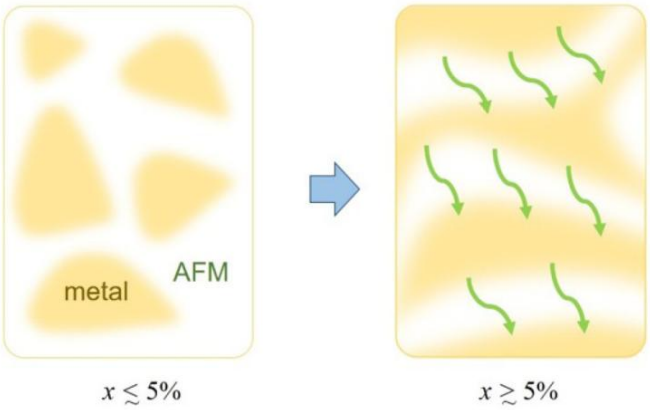

FIGURE 1. Schematic of possible electronic inhomogeneity for doping levels x <5% and x >5%.

References

1. Pelc, D., Grafe, H.-J., Gu, G. D., and Požek, M., *Phys. Rev. B* **95**, 054508 (2017).
2. Vučković, M., et al, *arXiv* 2405.18561v2 (2025)

Doped Infinite-layer Nickelate Superconductors and Tri-layer Nickelates: Self-consistent DFT+DMFT Approach

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Abstract. Infinite-layer superconducting nickelates, RNiO$_2$ (R = La, Nd, Pr), and more recently the tri-layer nickelates have garnered interest in the field in the hopes of a better understanding of unconventional superconductors. Study of the normal state is paramount to the understanding of the state out of which superconductivity emerges and possibly the mechanism and symmetry of the pairing state. Properties of these novel class of materials are expected to be influenced by the presence of correlated d and/or f-electrons. Large-scale first-principle computational approaches can be valuable in deciphering experimental findings and predicting results. We present results of our recent self-consistent DFT + DMFT work on undoped nickelate superconductors, as well as, ongoing work on the doped systems. We propose a correlation-temperature (U-T) phase diagram for the undoped nickelates, showing low-T Fermi liquid phases (partially screened and fully screened nickel d-electron moments), a high-T Curie-Weiss phase of fluctuating nickel d-electron moment, and an antiferromagnetic phase at large U. To describe physics at non-zero doping, we carry out DFT + DMFT calculations on supercells appropriate to respective dopings, for a given correlation strength, and across a wide range of temperature. Our results indicate consequential departure from the undoped system, including possible Ni-site-selective behavior in scattering rate, spin susceptibility and spectral function. This may have consequences for superconductivity. We also present results of similar calculations on the tri-layer nickelates.

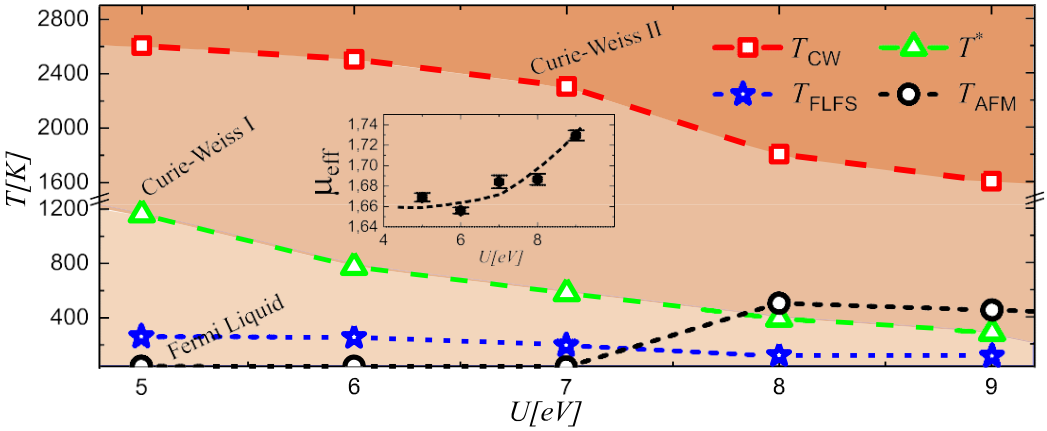

FIGURE 1: Proposed Correlation-temperature phase diagram of undoped nickelate

Animal Respiratory Viruses with Zoonotic Potential

Andrea Radalj[a], Marko Janković[b], Stefan Mijatović[b], Irena Aranđelović[b], Anđelija Ilić[c], Mira Aničić Urošević[c], Jelena Trajković[c], Jelena Ajtić[a], Stefan Đoković[a], Predrag Kolarž[c]

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Abstract. Respiratory viruses of animal origin pose a major public health risk due to their ability to cross species barriers and cause zoonotic infections. Influenza A viruses, especially those from avian and swine hosts, have driven several human pandemics [1]. Their segmented genome enables genetic reassortment, leading to antigenic shifts and the emergence of novel human-infecting strains. Swine act as "mixing vessels" for avian, human, and swine influenza viruses, increasing pandemic risk. Similarly, HPAI H5N1 causes sporadic, often fatal human infections linked to contact with infected poultry [2]. Coronaviruses such as SARS-CoV, MERS-CoV, and SARS-CoV-2 likely originate from bats, with spillovers involving intermediate hosts like civets or camels. SARS-CoV-2, probably arising from a wildlife market, sparked a global pandemic with severe health and socio-economic effects [1,3]. These events highlight the need for animal surveillance, viral evolution research, and a One Health approach to prevention and control.
Acknowledgement. This work has been supported by The Science Fund of the Republic of Serbia, Green program of cooperation between science and industry, grant no. 5661, project acronym – IonCleanTech.

FIGURE 1. Coronaviruses and influenza viruses with zoonotic potential and the One Health approach.

REFERENCES

1. Radalj, A., and Nišavić, J., "Some Viral Infections of Animals as a Potential Public Health Risk" in FEMS Online Conference on Microbiology, 2020, p. 17.
2. Khalil, A.M., Martinez-Sobrido, L., and Mostafa, A., *Front. Cell. Infect. Microbiol.* **13**, 1232772 (2024).
3. Nišavić, J., Milić, N., and Radalj, A., *Vet. Glas.* **74,** 1-17 (2020).

Structure-Property Relationships in Oxide Ion Conductors for Energy Applications

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Abstract. An in-depth understanding of the structure – property relationships is essential for the discovery and development of new functional materials capable of overcoming the limitations of the currently used ones. This presentation will give an overview of our work on the development of oxide ion conductors, some of which are the best-in-class performing materials. It will cover the elucidation of key design principles, defects and mechanisms giving rise to ionic mobility; the development and use of advanced structural data analysis methodologies capable of tackling exceptionally complex crystallographic problems arising from phase transitions; the complementary use of long-range and local structural probes in understanding the structure, disorder and properties. In addition, it will illustrate the understanding of the oxide-ion dynamics in solid electrolytes which quasielastic neutron scattering, supported by ab-initio molecular dynamics calculations, can provide. Examples will include ionic conductors from several different structural families, such as fluorite [1, 6], apatite [3] and perovskite-related [2, 4, 5] materials.

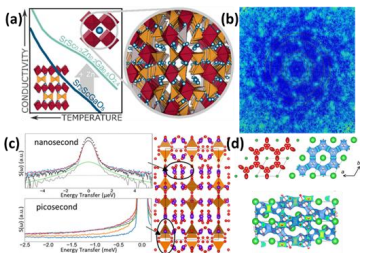

FIGURE 1. (a) Composition – structure – property relationships in oxygen-deficient perovskites. (b) Single crystal neutron diffuse scattering from a disordered apatite-type silicate. (c) QENS signatures of the oxide ion dynamics in a bismuth vanadate with fluorite-type superstructure. (d) Relationships between structure, ADPs and ionic migration pathways in a hexagonal perovskite-related oxide ion conductor.

REFERENCES

1. Schwaighofer, B., Gonzalez, M. A., Appel, M., Koza, M. M & Evans, I. R. (2023). *Chem. Mater*., **35**, 3, 1125.
2. Fuller, C. A., Murrell, J. I., Blom, D. A., Vogt, T., Zhang, W. Halasyamani, P. S., Evans, I. R. & Evans, J. S. O. (2022). *Chem. Mater*., **34,** 7, 3185.
3. Fuller, C. A., Gutmann, M. J., Ling, C. D., Wang, C. H., Zhang, W. Halasyamani, P. S., Evans, I. R. & Evans, J. S. O. (2022). *J. Mat. Chem. A*, **10**, 27, 14576.
4. Fuller, C. A., Blom, D. A., Vogt, T., Evans, I. R. & Evans, J. S. O. (2021). *J. Amer. Chem. Soc*., **144,** 1, 615.
5. Auckett, J. E., Milton, K. L. & Evans, I. R. (2019). *Chem. Mater*., **31**, 5, 1715.
6. Peet, J. R., Fuller, C. A., Frick, B., Koza, M. M., Johnson, M. R., Piovano, A. & Evans, I. R. (2019). *J. Amer. Chem. Soc*., **141,** 25, 9989.

Writing Successful Proposals for Beamtime at Large Facilities: Before, During and After the Experiment

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Abstract. This presentation will cover the entire cycle of working with large scale user facilities: experiment planning and writing successful beamtime proposals, performing the experiment and post-experiment activities such as report writing and publication of results. These aspects will be covered in general, but also in the specific contexts of accessing neutron and synchrotron facilities for studies of structure and dynamics of functional materials across the chemical spectrum.

Tunable Electronic States: Semiconductor-to-Metallic state Transition in CeO_2 Nanocrystals

Marko Radovic

Center for Sensing Technologies, Biosense Institute, Novi Sad, Serbia

Abstract. This study harnesses advanced optical spectroscopy to decode the mechanisms governing the insulator-to-metal transition (IMT) in lanthanide oxides, with a focus on CeO_2 nanocrystals. We bridge the gap between bulk material properties and emergent nanoscale phenomena, revealing how heavy doping (Fe^{3+}, Nd^{3+}) and quantum confinement synergistically drive metallicity. Using Raman, IR, and spectroscopic ellipsometry as nanoscale probes, we track the interplay of electronic and vibrational dynamics. Raman spectroscopy captures the F_2g mode softening and broadening under Fe^{3+} doping, linking these shifts to free-carrier screening and electron-phonon coupling. IR spectroscopy identifies plasmon-phonon hybrid modes in Nd-doped nanocrystals, a hallmark of the semiconductor-to-metallic state crossover. Spectroscopic ellipsometry maps the bandgap evolution, revealing a paradoxical Burstein-Moss-driven widening concurrent with metallization. Our findings culminate in a revised band structure model for CeO_2 nanocrystals, visualizing the IMT as a function of doping and size. This work not only establishes optical spectroscopies as indispensable tools for probing quantum phase transitions but also opens avenues for designing tunable optical materials for semiconducting technologies, photonic devices and sensors.

Spectroscopy at the Synchrotron, Microscopy of the Quantum World

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Abstract. Understanding the properties of quantum materials, such as strongly correlated electron systems, topological materials, and unconventional superconductors, requires advanced experimental techniques capable of probing their fundamental nature. **Angle-Resolved Photoemission Spectroscopy (ARPES)** [1] and **Resonant Inelastic X-ray Scattering (RIXS)** [2] are two powerful synchrotron-based techniques that provide complementary insights into the electronic structure and excitation spectra of these materials.

ARPES is an established method for directly mapping the electronic band structure of materials with momentum resolution, offering detailed insights into Fermi surface topology, electron correlations, spin-orbit coupling effects, and low-energy quasiparticle phenomena.

RIXS, on the other hand, is a highly sensitive probe of charge, orbital, spin, and lattice excitations, enabling a deeper understanding of the many-body interactions governing quantum materials. Additionally, by tuning the incident X-ray energy to a specific absorption edge, RIXS provides element- and orbital-specific information on collective excitations, including spin waves (magnons), phonons, and charge-ordering phenomena.

At modern synchrotron facilities, advancements in beamline instrumentation, high-resolution detectors, and improved sample environments have significantly enhanced both techniques, allowing for ***in situ*** studies of emergent quantum phases.

In my talk, I will present several examples demonstrating the capabilities of ARPES [3, 4] and RIXS [5] in understanding and uncovering novel phenomena in quantum materials.

REFERENCES

1. Sobota, J. A., and He, Y., and Shen, Z-X., Rev. Mod. Phys. **93**, 025006 (2021).
2. Mitrano, M. and Johnston, S., and Kim, Y-J., 4 and Dean, M. P. M., Phys. Rev. X **14**, 040501 (2024).
3. Caputo, M., et al., Advanced Science 8 (19), 2101516 (2021).
4. Li, H, et al., Advanced Functional Materials **34**, 2313236.
5. Asmara, T. C., et al., Advanced Materials **36**, 2310668 (2024).

The use of differential photocurrent in the characterization of novel optically active materials

Louisa Reissig

Freie University Berlin

Abstract. Transferring information through the use and detection of light signals is a cornerstone of modern technology and thus a large number of studies is devoted to characterising the optical and opto-electronic properties of novel materials. Novel inorganic and organic materials are synthesised and their light-sensitivity optimised through e.g. structural changes on the nano-range. Furthermore, with the increasing shift to "green" consumer electronics, attention has also been directed towards bio- or bioinspired materials and strategies.

While developing a novel photodetecting architecture [1], we recently uncovered the devices potential in screening and characterising the optical and opto-electronic properties of a range of materials, such as photoactive proteins [2], functionalised 2D materials [3], as well as inorganic thin films comprising semiconductor or ferroelectric materials. In this talk I will present the resent developments in the field of photodetection, where e.g. the integration of proteins can add secondary functionalities to the devices. Furthermore, I will provide an overview of how the differential photocurrent technique, in combination with the soft on-tip-on-dip architecture [4], can be used for screening optically active materials with high resolution, irrespective of the degree of transparency and reflectivity of the sample, I will comment on the ease of performing such screening experiment and present intriguing recent results.

REFERENCES

1. L. Reissig, S. Dalgleish, K. Awaga *A differential photodetector: Detecting light modulations using transient photocurrents* AIP Advances **6(1):015306** 2016 DOI:10.1063/1.4939921
2. L. Reissig, K. Buchanan, Th. Lindner, M. Kurihara, P.-Ch. Chan, F. Kibowski, K. Kojima, S. Dalgleish, K. Awaga, Y. Sudo *The use of microbial rhodopsin proteins in differential photodetection* Frontiers in Physics: Optics and Photonics **12** 2024 DOI:10.3389/fphy.2024.1481341
3. N. Mutz, S. Park, Th. Schultz, S. Sadofey, S. Dalgleish, L. Reissig, N. Koch, E. List-Kratochvil, S. Blumstengel *Excited-state charge transfer enabling MoS2/Phthalocyanine photodetectors with extended spectral sensitivity* Journal of Physical Chemistry C **124(5):2837–2843** 2020 DOI:10.1021/acs.jpcc.9b10877
4. S. Dalgleish, L. Reissig, Y. Sudo, K. Awaga *On-Tip Photodetection: A Simple and Universal Platform for Optoelectronic Screening* Chemical Communications **51(91):16401-16404** 2015 DOI:10.1039/c5cc06237c

Charge density waves and superconductivity in Vanadium based Kagome metals

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Abstract. Materials hosting Kagome lattices are of great interest due to their unique electronic structures, which feature flat bands, Dirac cones, and non-trivial band topology, providing a unique platform for exploring novel collective quantum states [1]. In this talk, we present a comparison of pressure and temperature-dependent X-ray diffraction studies on two prominent members of this material family, namely CsV_3Sb_5 and ScV_6Sn_6, focusing on their electronic superlattices and their relation to superconductivity. Our study on CsV_3Sb_5 reveals a pressure-induced transformation of the charge density wave (CDW) pattern from a 2 × 2 structure to a commensurate 3/8 modulation near 0.7 GPa and a full suppression of the electronic order above 2GPa, which correlates with anomalies in the superconducting transition temperature (see Fig. 1) [2]. In contrast, the response of ScV_6Sn_6 to similar conditions is very different. By comparing these two systems, we aim to elucidate the role of lattice distortions and CDW fluctuations in enhancing or suppressing superconductivity in kagome materials.

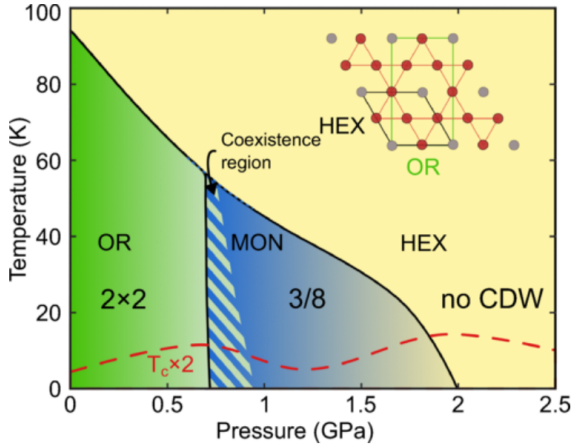

FIGURE 1. Electronic phase diagram of CsV3Sb5 in the low-pressure and low-temperature region. The orthorhombic 2×2×2 and 2×2×4 phases, summarized as 2×2, exist in the green region below ≈ 0.7 GPa. The new monoclinic phase with the 3/8 order is indicated in blue.

REFERENCES

1. T. Neupert, et al., Nat. Phys. 18, 137 (2022).
2. F. Stier,..., T. Ritschel, et al., Physical Review Letters 133, 236503 (2024).

Art Restoration and Science: A Brief History of Entanglement

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Abstract. The field of conservation and restoration of artworks has greatly advanced through the integration of scientific methodologies. By bridging the gap between science and art, conservators gain deeper insights into the materials, techniques, and causes of deterioration that affect artworks. The recognition of artworks as cultural heritage and the need for their preservation can be traced back to the Renaissance. Questions regarding the authenticity of artworks, ethical considerations in restoration, and the compatibility of original materials with those used in restoration began to emerge. These concerns are exemplified by the restoration approaches applied to *The Laocoön Group* sculpture and the Parthenon temple [1]. Among different art forms, wall paintings, due to their monumental nature and direct exposure to environmental and human factors, are particularly reliant on scientific advancements for effective preservation. Techniques such as X-ray fluorescence (XRF), and Raman spectroscopy are widely used to identify pigments and binding media employed by original artists. A notable domestic example of such scientific application occurred during the conservation of wall painting fragments from villa at the archaeological site Mediana, conducted at the Faculty of Applied Arts in collaboration with the Institute for the protection of cultural monuments and Faculty of Physics, Belgrade. Scientific analyses revealed the use of the pigment vermilion. Given that vermilion was very expensive pigment used by the Romans, and its price was fixed by the government [2] this discovery suggests that Mediana held significant importance. Consequently, these findings reshape the historical understanding of the entire archaeological site. By combining analytical techniques, science not only reveals the artworks past, but also protects them for the future.

REFERENCES

1. Jokileto, J., A History of Architectural Conservation, The University of York, Institute of Advanced Architectural studies, 1986, pp 11-37, 149-162.
2. Gettens, J. R., Stout L.G., “Painting Materials, A Short Encyclopaedia” New York: Dover Publications, 1942, pp 171-173.

Elasticity of Charge Density Wave Superlattice in Low-dimensional Materials

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Abstract. Although the modulation of charge density in lattices, i.e. charge density wave (CDW), was first proposed by Peierls as an instability in one-dimensional (1D) metal, recent studies have revealed diverse origins of the CDW in real materials. The generalization of the previously more narrowly-defined concept of CDW calls for a revisit of signatures of CDW established in early studies of CDW physics. One of the key signatures of the CDW is the finite elasticity of its superlattice. Early studies of the elasticity of CDW superlattice have mostly been focused on quasi-1D materials, mainly in the bulk form, experiments revealing the elasticity of higher-dimensional CDW materials are scarce, and the finite size effect on the CDW elasticity remains unclear. In this talk, I will discuss our recent work on the studies of elasticity of CDW at higher dimensions [1] and in nanodevices [2], and on the elastic-plastic transition of the CDW superlattice [3], using transport measurements and noise spectroscopy. If time permits, I will also discuss the development of some other experimental techniques in extreme conditions and their applications in studying quantum materials in our group.

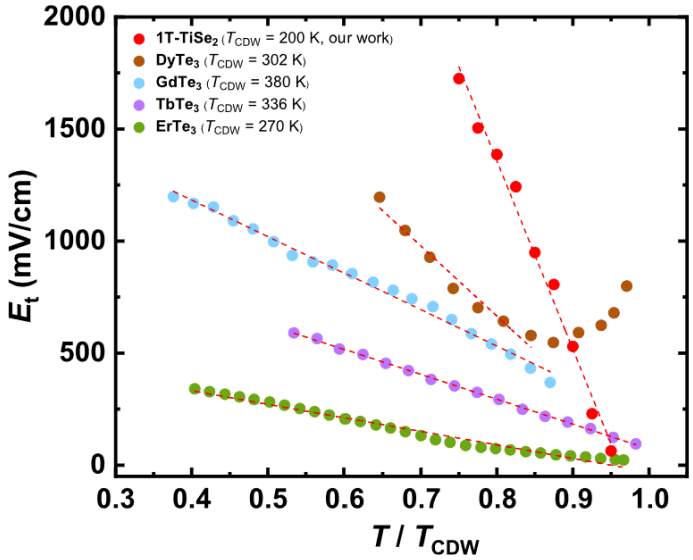

FIGURE 1. Threshold electric field $E_T(T)$ in 2D CDW systems, including 1T-$TiSe_2$ [1] and $DyTe_3$ [4], $GdTe_3$ [5, 6], $TbTe_3$ [5, 6], $ErTe_3$ [7].

REFERENCES

1. X. Wei, L. Zhu, Z. Wu, Zhenzhong Shi, *J. Phys.: Condens. Matter*. **36**, 485501 (2024).
2. Zhenzhong Shi, L. Zhu, P. M Marley, K. Farley, S. Banerjee, G Sambandamurthy, *New J. Phys.* **26** 123002 (2024).
3. L. Zhu, Z. Wu, Zhenzhong Shi, In preparation.
4. A. A. Sinchenko, P. Lejay, P. Monceau, *Phys. Rev. B* **85**, 241104 (2012).
5. A. A. Sinchenko, P. Lejay, O. Leynaud, P. Monceau, *Solid State Commun.* **188**, 67 (2014).
6. A. Sinchenko, P. D. Grigoriev, P. Lejay, O. Leynaud, P. Monceau, *Physica B* **460**, 21 (2015).
7. A. A. Sinchenko, P. Lejay, O. Leynaud, P. Monceau, *Phys. Rev. B* **93**, 235141 (2016).

Uncovering the Hidden Ferroaxial Orbital Density Wave as the Origin of the Axial Higgs Mode in RTe_3

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Abstract. Detecting unconventional density waves and identifying their underlying mechanism has proven particularly challenging. Here, I will discuss our discovery of a rare ferroaxial CDW order from orbital modulation requiring a nontrivial order parameter. Using Raman spectroscopy and quantum interference, we revealed the first axial Higgs mode [1] associated with charge order. Additional Raman, Rotational-Anisotropy Second-Harmonic Generation, and Scanning Transmission Electron Microscope experiments establish this occurs in a density wave that breaks all vertical and diagonal mirror symmetries, while preserving the spatial inversion. The Raman and μSR experiments further confirm the absence of time-reversal symmetry breaking [2]. Simultaneously, Raman scattering shows the CDW produces a Higgs mode and the electronic Raman response from the CDW gap with axial symmetry across the rare-earth tritellurides family. I will discuss how this can be explained by a rare combination of orbital and charge order that results from the unique quantum geometry of the rare-earth tritellurides.

REFERENCES

1. Wang, Y., et al., *Nature* **606**, 896-901 (2022).
2. Singh, B., et al., *arXiv*:2411.08322v2 (2024).

Harnessing Heat: The Dynamic World of Thermosalient Materials

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Abstract. The thermosalient effect, characterized by the abrupt mechanical motion of crystals in response to thermal stimuli, represents a fascinating phenomenon in materials science. This effect occurs due to thermal single crystal to single crystal phase transitions and anisotropic lattice expansion/contraction at the microscopic scale, resulting in macroscopic behaviors such as jumping, bending, or rotation of crystals. The importance of the thermosalient effect lies in its potential to convert thermal energy into mechanical work, making it a promising candidate for various applications. These include the development of actuators, sensors, and energy harvesting devices. The ability of thermosalient materials to undergo rapid and reversible shape changes without the need for external power sources positions them as key components in the design of smart materials and soft robotics.

Despite their potential, several challenges hinder the practical application of thermosalient materials. One major challenge is the fixed nature of their phase transition temperatures, which limits their adaptability to different environments. Additionally, the mechanical stress induced during the phase transition can lead to the fragmentation of crystals, reducing their durability and reliability.

Addressing the challenges associated with these materials will be essential for unlocking their full potential in various applications. This presentation aims to explore recent advancements and future directions in thermosalient materials research.

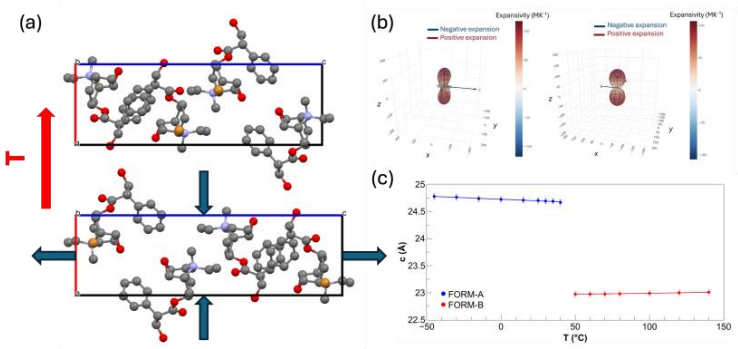

FIGURE 1. a) Unit-cell of oxitropium bromide (OXTB) form A and B; b) thermal expansivity indicatrix of OXTB form A and B; c) unit-cell parameter *c* of OXTB form A and B

1. Skoko, Ž., Zamir, S., Naumov, P., Bernstein, J., *J. Am. Chem. Soc.* **132**, 14191–14202 (2010).
2. Lončarić, I., Popović, J., Despoja, V., Burazer, S., Grgičević, I., Popović, D., Skoko, Ž., *Cryst. Growth Des.*, **17**, 4445–4453 (2017)
3. Klaser, T., Stepančić, O., Popović, J., Pisk, J., Pavić, L., Picek, I., Matković-Čalogović, D., Skoko, Ž., *J. Mater. Chem. C*, (2025), doi: 10.1039/d4tc04615c

Novel 2D magnets and dielectrics

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Abstract. The recent progress in methods of high quality and low defect 2D magnetic materials will be discussed. Beside the group of transition metal halides and chalcogens also the rapidly growth family of mixed halogen-chalcogenides will be introduced. The dominantly explored material, chromium sulfo-bromide adopt FeOCl structure and possess A type antiferromagnetic ordering at low temperature. By various methods of exfoliation or defect formation, this material can be converted to ferromagnetic state. The chemistry of CrSBr including doping and possible covalent and non-covalent functionalization and its effect on magnetic and optical properties will be presented together with possible applications in electronic devices [1]. Beside the two dimensional magnets, the 2D dielectric exhibit important group of materials with crucial rule in device fabrication. The broad spectra of novel high-k 2D dielectric materials growth and applications will be presented together with large scale crystal growth of hexagonal boron nitride at atmospheric pressure using various metal flux.

REFERENCES

1. K. Mosina, B. Wu, N. Antonatos, J. Luxa, V. Mazánek, A. Söll, D. Sedmidubsky, J. Klein, F. M. Ross and Z. Sofer, *Small Methods* **8**, 2300609 (2024).

Strain Engineering in hBN/$M^{III}X^{VI}$ Heterostructures for Enhanced Optoelectronic Performance

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Abstract. Group IIIa monochalcogenides ($M^{III}X^{VI}$, M = Ga, In; X = S, Se, Te) are promising 2D materials due to their high electron mobility, tunable bandgaps, and strong light absorption. However, their chemical sensitivity, particularly oxidation in ambient conditions, limits their stability and device integration. Encapsulation with hexagonal boron nitride (hBN) provides an effective solution, offering both mechanical protection and enhanced electronic and optical properties [1]. This study investigates the structural, electronic, and optical properties of hBN/$M^{III}X^{VI}$ heterostructures (HS), with a particular focus on the role of mechanical strain in tuning their performance. Using biaxial strain, we demonstrate precise bandgap modulation and improved optical absorption while preserving material symmetry [2,3]. Our results highlight hBN/InTe and hBN/GaTe as particularly promising HSs due to their excellent lattice matching, enhanced mechanical stability, and broad-spectrum absorption in the visible range [2]. These findings not only advance fundamental understanding of strain-engineered HSs but also provide design strategies for integrating these materials into next-generation optoelectronic devices, including flexible photodetectors and absorbers.

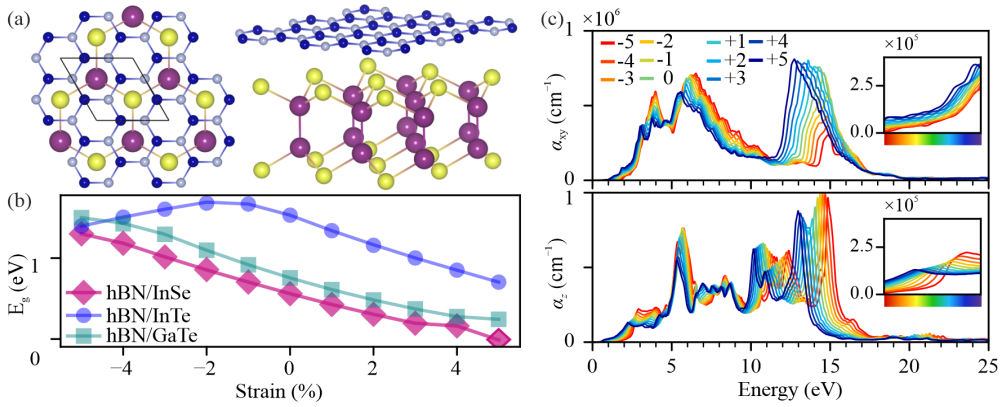

FIGURE 1. (a) Top and side view of hBN/$M^{III}X^{VI}$ HS, (b) calculated bandgap of hBN/InSe, hBN/InTe and hBN/GaTe for different strain intensities, (c) Absorption of hBN/GaTe HS under strain.

REFERENCES

1. Šolajić, A., Pešić, J., *Journal of Physics: Condensed Matter.* **34(34)**:345301, 2022.
2. Šolajić, A., Pešić, J., *Scientific Reports*, **14(1)**:1081, 2024.
3. Šolajić, A., Pešić, J., *Optical and Quantum Electronics*, **56(7)**:1186, 2024.

Superconducting Properties of Borophenes from First Principles

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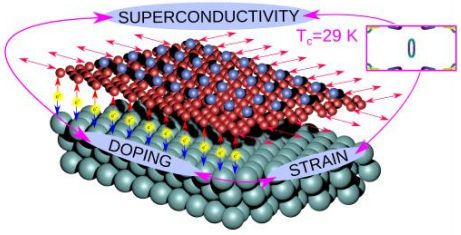
Abstract. With outstanding physical and chemical properties, borophene - a 2D allotrope of boron - offers greater application potential than graphene [1]. However, its susceptibility to oxidation under ambient conditions remains a challenge [2], which can be mitigated through hydrogenation of monolayer [3] or fabrication of bilayer configurations [4]. Using first-principles simulations and solving the anisotropic Migdal-Eliashberg equations, we demonstrate that these two configurations are promising superconducting candidates, with the hydrogenated monolayer reaching a superconducting critical temperature (T_C) of 29 K [5], and alkaline-earth metal-intercalated bilayers reaching T_C up to 58 K [6]. Our results also resolve the long-standing question of why bare monolayer borophene lacks superconducting properties, consistent with the absence of experimental evidence. Furthermore, we show how hydrogenation enhances its superconducting properties and how bilayer intercalation enables further tunability, bridging a critical gap in the search for practical boron-based superconducting devices.



REFERENCES

1. Prashant Kumar *et al.*, *Progress in Materials Science*, **146**, 101331 (2024).
2. Xiaolong Liu *et al.*, *Nanotechnology*, **33**, 235702 (2022).
3. Qiucheng Li *et al.*, *Science*, **371**, 1143-1148 (2021).
4. Caiyun Chen *et al.*, *Nature Chemistry*, **14**, 25-31 (2022).
5. Božidar N. Šoškić *et al.*, *Nano Letters*, **24**, 12650-12657 (2024).
6. Božidar N. Šoškić *et al.*, *Physical Review Materials*, **8**, 064803 (2024).

Laser-Induced Graphene on Polymer Substrates for Monitoring Physiological Parameters

Marko Spasenović[a], Teodora Vićentić[a], Anđela Gavran[a], Vanja Vojnović[a], Katarina Tošić[a], Milena Rašljić-Rafajilović[a], Stefan Ilić[a], Marija V. Pergal[a]

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Abstract. Laser-induced graphene (LIG) is a versatile platform with applications in sensing of physiological parameters, electrodes, gas sensors, and biosensors [1, 2]. However, most LIG research has focused on rigid substrates as well as those that are not biocompatible, which would be important for applications that require direct contact between the sensor and skin. To address this limitation, we present a novel approach: laser induction of graphene on biocompatible synthesized cross-linked polymers, including sodium alginate, poly(dimethylsiloxane)/poly(ethylene glycol) (PDMS/PEG) composites, cross-linked polyurethanes (PUs) based on ethoxypropyl terminated PDMS macrodiol, and synthesized polyimides. The synthesized cross-linked polymers with good mechanical properties, non-cytotoxic chemistry, and good biocompatibility, are good candidates for wearable sensors. Our study identifies optimal chemical compositions and laser processing parameters for LIG on these biocompatible substrates. We demonstrate the practical application of LIG-based wearable patches for sensing heartbeat, human respiration, and limb motion. Our results pave the way for developing novel biocompatible, unobtrusive, cost-effective, and efficient thin-film LIG sensors for continuous monitoring of physiological parameters.

This research was supported by the Science Fund of the Republic of Serbia, #4950, Polymer/graphene heterostructures for physiological sensors – Polygraph.

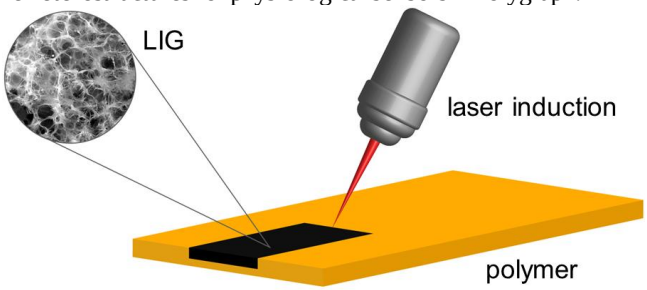

FIGURE 1. Representation of Laser Induction of Graphene on Polymer Substrate.

REFERENCES

1. Wang, M., Yang, Y., and Gao, W., *Trends Chem.* **3,** 969-981 (2021).
2. Vićentić, T., et al, *Sensors* **22**, 6326 (2022).

Experimental Chemotherapy of Reactivated Toxoplasmosis

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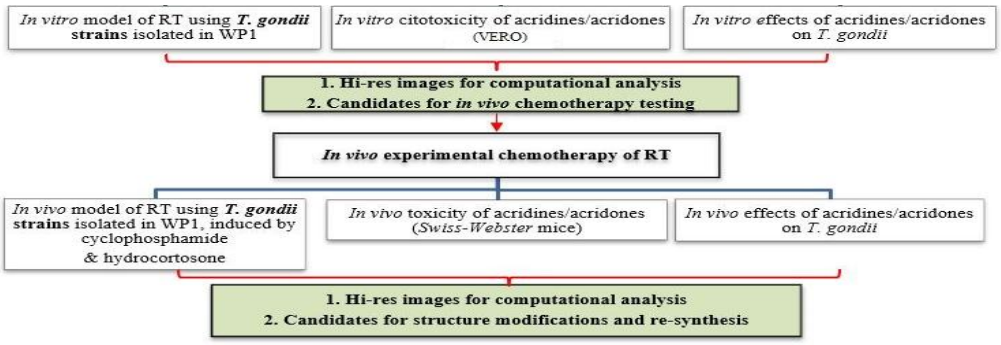
Abstract. Reactivated toxoplasmosis (RT) is a consequence of severe immunosuppression in individuals chronically infected with the parasite *Toxoplasma gondii*. Newly synthetized and modified acridine and acridone derivatives will be investigated in both *in vitro* and *in vivo* RT model systems. For *in vitro* models *T. gondii* strains were propagated in Vero cell line, while cell toxicity effects of treatment as well as determination of IC_{50} values were evaluated by MTT assay and parasite viability assay [1]. *In vivo* efficacy of derivatives selected on the basis of their *in vitro* results will be investigated in murine models of acute, chronic and RT induced by immunosuppressants commonly used in hematopoietic stem cell transplantation (HSCT) patients - cyclophosphamide and corticosteroids [2]. **Acknowledgement**. This research was funded by the Science Fund of the Republic of Serbia, 7328, Reinvention of the diagnostic algorithm and treatment options for reactivated toxoplasmosis—ToxoReTREAT.



SCHEME 1. Experimental chemotherapy of reactivated toxoplasmosis

REFERENCES

1. Zlatković, Đ., Dobričić, V., Srbljanović, J., *et al., Pharmaceutics 17(3), 374* (2025).
2. Bauman, N., Srbljanović, J., Čolović Čalovski, I., *et al., Fractal Fract 8(3), 175* (2024).

Reinvention of the diagnostic algorithm and treatment options for reactivated toxoplasmosis – ToxoReTREAT project

Tijana Štajner[a], Jelena Srbljanović[a], Olivera Lijeskić[a], Đorđe Zlatković[a], Srđan Pašić[b,c], Borko Gobeljić[c], Marija Simić[c], Vladimir Dobričić[d], Jelena Trajković[e,f], Andjelija Ž. Ilić[e], Branko Bobić[a]

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Abstract. *Toxoplasma gondii* infects nearly a third of the global population, posing a serious risk to immunosuppressed individuals, especially after allogeneic hematopoietic stem cell transplantation (allo-HSCT) [1]. Despite increasing number of HSCT procedures in Europe, standardized monitoring and treatment guidelines for reactivated toxoplasmosis (RT) are lacking. Current treatments are toxic and ineffective. The ToxoReTREAT project aims to improve RT diagnostics, treatment, and cost-effectiveness through a multidisciplinary approach. Molecular monitoring of allo-HSCT recipients and risk factor analysis will enable refinement of diagnostic algorithm and National guidelines development. Newly synthesized acridine and acridone derivatives are tested in experimental RT models, while ImageJ software automates and enhances chemotherapy assessment. The project's ultimate goal is to identify a safer, more effective treatment options for RT. **Acknowledgement**. This research was funded by the Science Fund of the Republic of Serbia, 7328, Reinvention of the diagnostic algorithm and treatment options for reactivated toxoplasmosis—ToxoReTREAT.

FIGURE 1. ToxoReTREAT project logo

REFERENCES

1. Štajner T, Vujić D, Srbljanović J, et al., *Clin Microbiol Infect* 28(5): 733.e1-733.e5 (2022).

Photon Condensation and Electromagnetic Response in Single Molecule Antiferromagnets with Flux Coupling

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Abstract. Photon condensation or superradiant phase transition was predicted to occur in a variety of models describing a collection of emitters collectively coupled to a mode of electromagnetic radiation. Just as often, a version of no-go theorem has predicted that such a transition can not occur. Current understanding is that a unique phase transition does occur, but its nature is gauge dependent. The transition appears either as a macroscopic occupation of the field mode that couples to emitters, or as a phase transition in the state of emitters. Observables that signify the transition are the state of the field in one gauge, and macroscopic polarization of emitters in the other. Relevance of the description in a given gauge is determined by the measurement that determines the system's state. We study photon condensation transition in a molecule that couples to the field through its flux. The simplest spinfull model of a molecule that shows nontrivial coupling of this type is a spin triangle. At zero temperature, the ground state of coupled molecule-radiation system is determined by the symmetry of the molecule and intensity of the coupling. In the case of a molecule with full symmetry of equilateral triangle, the transition does not happen and the ground state is always condensed, which corresponds to antiferromagnetic ground state with modifications of magnetic response due to photon condensate. With Jahn-Tellar or structural asymmetry, the transition appears at finite coupling strength of molecule to radiation. Resulting state shows modifications of both magnetic and electric response.

Role of terbium doping in controlling oxygen vacancies and enhancing conductive performance in $BiFeO_3$ thin films

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Abstract. The influence of Tb doping on structural and electrical properties of $BiFeO_3$ thin films is investigated, combining the experimental observations and density functional theory. With such an approach we aimed to elucidate the influence of Tb dopant and defects in the form of oxygen vacancies on electronic structure and electrical conductivity of $BiFeO_3$ films. X-ray diffraction confirmed that the rhombohedral (*R3c*) crystal structure remains stable in the whole doping range without any impurity phases. Relatively large leakage current was generated in pure $BiFeO_3$ and 5% and 20% Tb-doped films. Significant reduction of electrical conductivity was seen only in 10% Tb-doped film. Conductive atomic force microscopy (C-AFM) allowed us to investigate local electrical conduction properties at the microscale level. The 10% Tb doped film exhibited the smallest conductive surface confirming that this sample has the smallest conductivity, whereas the current maps revealed that the conduction takes place across spatially inhomogeneous grain boundaries with enhanced concentration of defects. The Raman and XPS measurements have shown that oxygen vacancies are the dominant defects in $Bi_{1-x}Tb_xFeO_3$ films. The higher concentration of oxygen vacancies, found in pure, 5% and 20% Tb-doped films can be responsible for higher conductivity of these films. A reduction in oxygen vacancy concentration was registered in 10% Tb-doped film which is in accordance with much lower conductivity of this sample. Density functional theory calculations provide atomic-level insights into the electronic transport mechanisms and are consistent with experimental findings. Undoped and low level Tb-doped samples (~5%) are conductive due to n-type dopants in the form of oxygen vacancies which are primarily localized on surface. For intermediate Tb doping (~10%), the balance between the effects of oxygen vacancies and dopant-induced states results in the highest electrical resistivity. Increased conductivity at higher doping levels (~20%) can be attributed to the denser population of Tb states around the Fermi level, which can overlap, presenting dispersive, conducting states. This work underlines the complex interplay of doping concentration, oxygen vacancies, and electronic transport, suggesting that 10% of Tb is an optimal dopant concentration for enhancing the electrical performances of $BiFeO_3$ thin films.

Surface Charge Density Wave in UTe2

Hermann Suderow[a]

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Abstract. UTe2 presents arguably one of the most intriguing superconducting phase diagrams, including superconductivity at extremely high magnetic fields and re-entrant and highly anisotropic behavior. Scanning Tunneling Microscopy (STM) measurements in UTe2 reveal intriguing properties, as a charge density wave (CDW), whose connection to the bulk is however difficult to establish. Here I will review atomic scale studies at surfaces of quantum materials, present recent developments in STM and show new measurements providing relevant features of the CDW in UTe2.

Precursors to Anderson Localization in the Holstein Model: Quantum and Quantum-Classical Solutions

Darko Tanasković

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Abstract. Weak van der Waals forces lead to strong thermal lattice fluctuations in molecular organic semiconductors. These fluctuations can be taken as a source of dynamic disorder and the charge transport is often described within phenomenological transient localization approach. Here we focus on the one-dimensional Holstein model near the adiabatic limit in order to make comparisons between the phenomenological and fully microscopical solutions. Recent methodological advances [1-2] enable us to solve the model at relevant temperatures and electron-phonon coupling. We find that the agreement between fully quantum and quantum-classical solutions is very good [3]. The most prominent feature is the appearance of a zero-frequency peak in the mobility, in addition to the displaced peak associated to the precursors of Anderson localization. The zero-frequency peak cannot be obtained within the phenomenological transient localization approach.

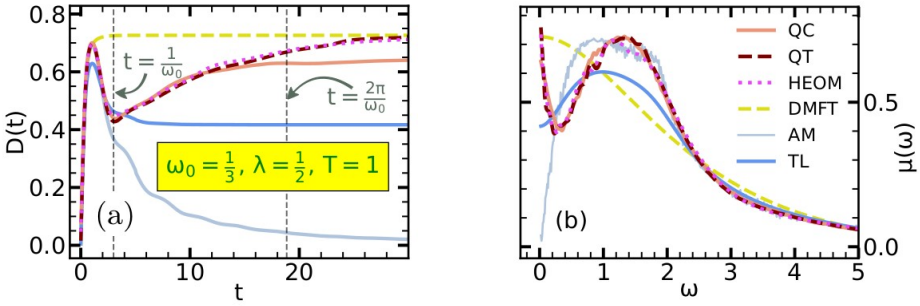

FIGURE 1. (a) Time-dependent diffusion constant. (b) Frequency-dependent mobility.

REFERENCES

1. V. Janković, P. Mitrić, D. Tanasković, and N. Vukmirović, Vertex corrections to conductivity in the Holstein model: A numerical-analytical study, Phys. Rev. B 109, 214312 (2024).
2. P. Mitrić, Dynamical quantum typicality: A simple method for investigating transport properties applied to the Holstein model, arXiv:2412.17436 (2024).
3. P. Mitrić, V. Janković, V. Dobrosavljević, and D. Tanasković, Precursors to Anderson localization in the Holstein model: Quantum and quantum-classical solutions, arXiv: 2412.17770 (2024).

Application Of Atomic Force Microscopy Based Techniques For Damage Assessment, Conservation, And Restoration Of Historical Papers And Fresco Wall Paintings

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Abstract. Two examples are presented how atomic force microscopy (AFM) and its derivatives can be employed for conservation of cultural heritage objects. In the first case [1], AFM topography investigation has been used to assess – in conjunction with Scanning electron microscopy – the damage of historic papers, mainly music, by a catastrophic fire in a 17th-century German library. In addition, the surface topography of the samples was studied after restoration treatment with commercial cellulose nanofibers (CNF). It could be demonstrated that CNF indeed stabilizes the partly burned sheet music. In an ongoing second case – within the framework of the Serbian Research Project "2DHeriPro" – we explore the possibility of utilizing two-dimensional materials like hexagonal boron nitride or ultrathin flakes of phyllosilicates to protect fresco wall paintings against external influences. Here, besides AFM topography measurements also Kelvin probe microscopy and AFM-based nanoindentation are used. In order to obtain chemical information on the nanometer scale, Photoinduced Force Microscopy as a nano-infrared (Nano-IR) tool is employed.

Work has been done in collaboration with Caterina Czibula, Lena Schwarz, and Markus Kratzer (all Montanuniversität Leoben, Austria), Laura Völkel and Antje Potthast (BOKU Vienna, Austria), and Tijana Tomašević-Ilić and Ivana Milošević (Institute of Physics, Belgrade, Serbia) as well as Bojana Savić (Faculty of Applied Arts, University of Arts, Belgrade, Serbia).

REFERENCES

1. L. Völkel, L.-S. Johansson, C. Czibula, M. Beaumont, D. Rusakov, A. Mautner, C. Teichert, E. Kontturi, T. Rosenau, A. Potthast, "Assessing fire-damage in historical papers and alleviating defects with soft cellulosic nanofibers", Small 18 (2022) 2105420-1-14. DOI: 10.1002/smll.202105420.

Inorganic nanotubes: From WS2 to "misfit" compounds

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Abstract. Update on the synthesis and characterization of new inorganic nanotubes from 2D compounds, like W(S,Se)21 will be given. The strong coupling between optical cavity modes confined in the nanotube and the exitonic transitions have been studied in some detail.1,2 Virtually recently, an "artificial recording eye" combining vison, storage and writing power has been established by a 4x4 array of WS2 nanotubes.3 Recent progress in mechanically reinforcing different polymers, will be briefly discussed.

Different nanotubes from quaternary "misfit" layered compounds (MLC) have been realized in recent years. In one recent case, the strong chemical affinity of the RE atoms towards sulfur atoms and that of selenium towards the tantalum atoms, led to the synthesis of highly anisotropic nanotubes, like RES-TaSe2 and RE-(TaSe2)2 (with RE=La, Sm) with extremely large (local) dipole moment.4 The high-temperature stability of such MLC nanotubes were studied with the help of synchrotron-based X-ray absorption and scattering techniques.5 Such nanotubes offer unique behavior, like 1D superconductivity, etc., suitable for quantum technologies.

REFERENCES

1. M.B. Sreedhara et al., *J. Am. Chem. Soc.* **144**, 23, 10530–10542 (2022).
2. S.S. Sinha et al., *Small* 2020, 16, 1904390 (2020).
3. Y. Sun et al., *Nature Comm.* **13**, 5391 (2022); https://doi.org/10.1038/s41467-022-33118
4. M.B. Sreedhara et al., *PNAS* **118**, 35 e2109945118 (2021).
5. A. Khadiev, M.B. Sreedhara, et al., *Acc. Chem. Res*. **57**, 3243-3253 (2024).

Tiled Network Films from Liquid Phase Exfoliated h-BN and Phyllosilicates: Properties and Perspectives for Heritage Protection

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Abstract. Nanotechnology approaches in conservation and restoration practices have enabled the development of advanced materials, offering promising solutions to mitigate the degradation of various artefacts [1–3]. Nevertheless, addressing the main conservation challenges with universal, durable, and cost-effective coatings, suitable for large-scale production remains an ongoing issue. As part of the 2DHeriPro project, we focused on exploring nanostructures beyond graphene-based materials to develop durable 2D material-based protective coatings for a broad range of heritage artefacts. We developed thin films from liquid-phase exfoliated (LPE) hexagonal boron nitride (h-BN), talc, and pyrophyllite, and systematically evaluated their potential for Heritage preservation. Our investigation encompassed an analysis of their chemical structure, optical properties, morphology, wettability, reversibility, and stability under conditions of high relative humidity, an oxidative environment, and thermal stress. Furthermore, to assess the compatibility of the films with wall-painting artefacts, we fabricated replica-models of fresco-paintings using colorimetry, spectroscopy, and morphology data obtained from heritage samples collected at relevant sites. These models, serving as substrates for the Langmuir-Blodgett (LB) deposition of 2D material-based films and the investigation of their compatibility, were produced from lime fresco mortar and identified pigments in order to reproduce the same color perception as the original artefacts. Although LB films from LPE h-BN with nanometer thickness exhibited superior transparency, hydrophobicity, and resistance to relative humidity and oxidation, colorimetric analysis of our films deposited on the model samples indicated that LPE talc-based films show the highest potential for application as coatings across diverse artefacts. In this presentation, we will outline the motivation, innovative approaches, and key findings from the first year of the 2DHeriPro project.

This research was supported by the Science Fund of the Republic of Serbia, Grant No 7456, 2D Material-based Tiled Network Films for Heritage Protection-2DHeriPro.

REFERENCES

1. Baglioni et al. *Molecules* **26**, 3967 (2021).
2. Kotsidi M. et al., *Nat. Nanotechnol*. **16**, 1004–1010 (2021).
3. Galvagno e. et al., *Adv. Funct. Mater*. **34** 2313043 (2024).

The Morphological And Structural Changes Of V_2O_5 Cathode Film Upon Electrochemical Cycling

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Abstract. Topics dealing with energy issues will always be of great importance. It has been known that vanadium oxide has potential application as a cathode material for the Li-ion batteries [1, 2]. The first step of this research is oriented towards designing the V_2O_5 thin film. For that purpose, the pulsed laser deposition technique [3] is used to deposit vanadium oxide thin film on a conductive substrate during heating at 400 ºC. Post annealing treatment is needed in order to achieve crystalline nature of V_2O_5 film. Besides the intention to evaluate the lithium storage capability of the oxide as a cathode, the aim is to thoroughly explore the changes occuring in the material during consecutive Li^+ insertion/deinsertion. The morphological and structural properties are investigated by Field Emission Scanning Electron Microscopy (FESEM), Atomic Force Microscopy (AFM) and Raman spectroscopy. Their correlation with the electrochemical performance is analyzed. The presented results will shed light on new insights into Li^+ storage mechanism of the vanadium oxide.

REFERENCES

1. Baddour-Hadjean, R., Pereira-Ramos, J.P., Navone, C., and Smirnov, M., *Chem. Mater.* **20**, 1916-1923 (2008).
2. Hevia, S. A., Orive, J., Guzman, F., Cisternas, E., Dietrich, F., Villarroel, R., and Lisoni, J., *Appl. Surf. Sci.* **576**, 151710 (2022).
3. Nag, J., and Haglund Jr, R. F., J. Phys.: Condens. Matter. **20** 264016 (14pp) (2008).

Carbon–Fiber and other Ionizer Types in Combating Airborne Pathogens – a Review

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Abstract. Airborne pathogens can cause infections, intoxications, or allergic reactions through respiration, dermal contact, or ingestion. Air ionization by dielectric barrier discharge or metal tip corona discharge produces ozone, a reactive ionization byproduct harmful to humans. This review focuses on the antimicrobial efficacy of newer carbon-fiber ionizers (CFIs) which can generate high ion concentrations, enhancing pathogen deposition, with almost negligible ozone production. Unipolar ions produced by the CFIs can disrupt microbial membranes, leading to cell death [1].
Acknowledgement. This work has been supported by The Science Fund of Serbia, Green program of cooperation between science and industry, grant no. 5661, project acronym IonCleanTech.

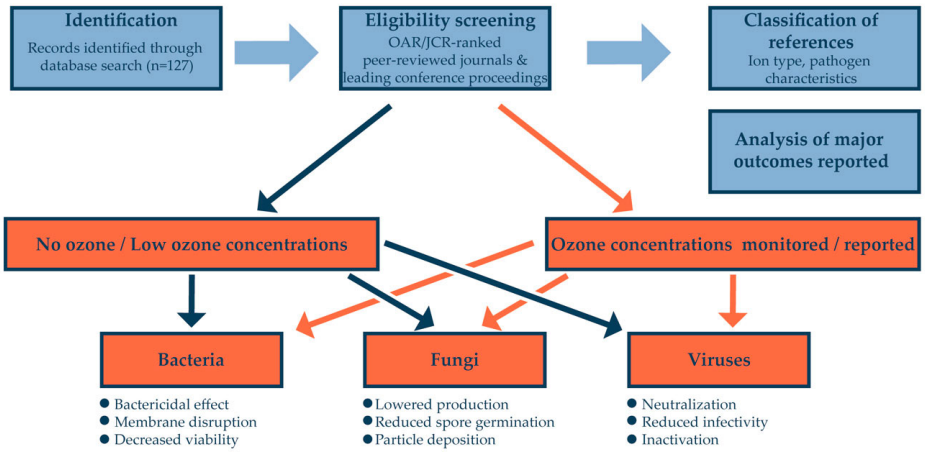

FIGURE 1. Search methodology and major data types used in the reference classification and evaluation. Major ionization outcomes. (Please see [1]).

REFERENCES

1. Radalj, A., Nikšić, A., Trajković, J., *et al.*, *Appl. Sci*. **14**(16), 7311 (2024).

Computational Image Analysis of Developmental Dynamics and Morphological Characteristics of Tachyzoites

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Abstract. Recently, we were among the first to apply computational image analysis in parasitology, and the first group to use fractal analysis to describe structural complexity of *Toxoplasma gondii* tissue cysts [1]. In this work, we study the *in vitro* conversion of bradyzoites to tachyzoites simulating reactivated toxoplasmosis (RT) in an immunocompromised host [2], and the effects of cellular invasion and intracellular proliferation (parasitophorous vacuole, rosettes, etc.).
Acknowledgement. This work was supported by the Science Fund of the Republic of Serbia through the PRIZMA Research Program (Project No: 7328, Project acronym: ToxoReTREAT).

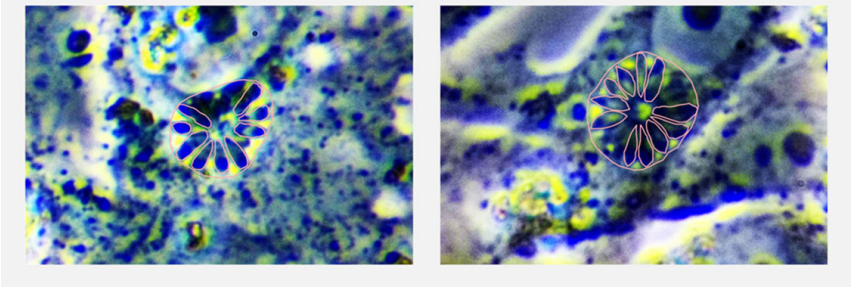

FIGURE 1. Photographs of example rosettes formed during the conversion of bradyzoites to tachyzoites in vitro.

REFERENCES

1. Bauman, N., Ilić, A., Lijeskić, O., *et al.*, *PLoS ONE* **15**(8), art.no. e0234169 (2020).
2. Rajnpreht, I., Klun, I., Uzelac, A., *et al*., *The 12th European Multicolloquium of Parasitology*, Turku, Finland, 20-24.07. 2016., eAbstract book O15.16.pdf (Oral presentation O15.16).

Portable Spectroscopic Instruments in Analyzing Art and Cultural Heritage: Advantages and Shortcomings

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Abstract. Portable spectroscopic instruments have transformed the analysis and conservation of artefacts and cultural heritage by enabling non-destructive in-situ examination. Techniques such as X-ray fluorescence (XRF), Fourier transform infrared spectroscopy (FTIR) and Raman spectroscopy provide useful insights into the composition and degradation of historical artefacts[1,2]. XRF facilitates elemental analysis, the differentiation of pigments and alloys [3], while FTIR[2] and Raman spectroscopy[4,5] are instrumental techniques indispensable in the identification of organic and inorganic compounds. These methods offer significant advantages, including rapid data acquisition, minimal risk of damage and complementarity with other analytical techniques[2]. However, they also have limitations such as limited sensitivity to certain elements, susceptibility to environmental influences and lower resolution compared to benchtop instruments[2,6]. Despite these shortcomings, their availability and efficiency make them indispensable in heritage science[7]. This lecture discusses the principles, applications, advantages, and limitations of these spectroscopic tools, presenting some case studies where they have been successfully applied in the conservation and study of cultural heritage. As technology advances, improvements in instrument sensitivity, miniaturization and data processing will further contribute to their application in cultural heritage studies, ensuring better preservation and a deeper understanding of historical artifacts[2].

FIGURE 1. Portable spectroscopic instruments in analyzing art and cultural heritage

REFERENCES

1. Bitossi, G., Giorgi, R., Mauro, M., Salvadori, B., and Dei, L., Spectroscopic Techniques in Cultural Heritage Conservation: A Survey, Appl. Spectrosc. Rev. 40, 187–228 (2005).
2. Pozzi, F., Rizzo, A., Basso, E., Angelin, E. M., de Sá, S. F., Cucci, C., and Picollo, M., "Portable Spectroscopy for Cultural Heritage," in Portable Spectroscopy and Spectrometry, edited by R. Crocombe, P. Leary, and B. Kammrath, Hoboken: John Wiley & Sons, 2021.
3. Shugar, A. N., and Mass, J. L., editors, Handheld XRF for Art and Archaeology, Leuven: Leuven University Press, 2012.
4. Vandenabeele, P., and Edwards, H., Raman Spectroscopy in Archaeology and Art History: Volume 2, Cambridge: The Royal Society of Chemistry, 2018.
5. Candeias, A., and Madariaga, J. M., "Applications of Raman Spectroscopy in Art and Archaeology," J. Raman Spectrosc. 50, 137–142 (2019).
6. Jehlička, J., and Culka, A., "Critical Evaluation of Portable Raman Spectrometers: From Rock Outcrops and Planetary Analogs to Cultural Heritage – A Review," Anal. Chim. Acta 1209, 339027 (2022).
7. Edwards, H., and Vandenabeele, P., Analytical Archaeometry: Selected Topics, Hoboken: RSC Publishing, 2012.

Microbial Assisted Biocontrol and Biocleaning In Stone Heritage Conservation – The Case of Rožanec Mithraeum Monument (Slovenia)

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Abstract. Fungi are considered one of the primary causes of deterioration of stone monuments worldwide, as well as a source of occupational hazard for conservators and restorers. Nowadays, implementation of novel, environmentally friendly methods for control of fungal infestation and restoration of incurred damages is gaining traction. Since the application of chemical biocides is increasingly discouraged due to toxicity, abrasiveness, promotion of resistance and non-selective mode of action, beneficial GRAS bacteria are investigated as the potential source of metabolites that would be appropriate alternative to overused chemicals. In this regard, bacteria of *Bacillus* and *Pseudomonas* genera were shown to be the most promising candidates due to a high yield of bioactive secondary metabolites, easy cultivation, and manipulation in the large-scale industrial reactors. In light of this, one of the main aims of the project "Novel biocides for cultural heritage of Southeast Europe–biocontrol and biomimetic systems for preservation of old masterpieces", as part of the planned conservation work on two deteriorated monuments in Serbia and Slovenia, was to bring to light all aspects of the autochthonous biofilm-induced formation of deterioration symptoms on the limestone Rožanec Mithraeum monument in the Judvoje forest in Slovenia. By combining numerous microscopic methods and state-of-the-art metabarcoding analysis, epilithic lichen *Gyalecta jenensis* and its photobiont, carotenoid-rich *Trentepohlia aurea*, were detected as the causative agents of salmon-hued pigmented alterations of limestone surface, while typical endolithic thalli and ascomata of representative Verrucariaceae family (*Verrucaria* sp.) together with the oxalic acid-mediated dissolution of limestone was behind the development of the main deterioration symptom on the monument, i.e., biopitting. In this way, a foundation was laid as the necessary prerequisite for further research on the development of biocontrol and biocleaning formulation for sustainable and long-term conservation of investigated stone monument. For this purpose, total non-culturable and culturable bacteriobiome of the monument were analyzed and isolated strains characterized for enzyme production, as a foundation of biocleaning process, and antifungal properties. *Bacillus mycoides* and *Paenibacillus amylolyticus* possessed the broadest enzymatic potential, while based on a broad spectrum antifungal activity, *Bacillus velezensis* and *Pseudomonas chlororaphis* subsp. *aurantiaca* were discovered as the most promising candidates for bacterial consortium effective in the treatment of deteriorated limestone monuments through joint activity. Bioformulations were efficient, lacked any corrosive effect, and proved safe for prolonged application when tested on laboratory models made from limestone obtained from the wall in the proximity of the Rožanec Mithraeum relief.

Electron and Lattice Dynamics During Transition to a Metastable Hidden State

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Abstract. Non-thermal phase transitions and hidden states in quantum materials hold great potential for novel applications, particularly when long-lived metastable phases are involved. A striking example is the light- or current-driven insulator-to-metal transition between charge-ordered states in 1T-TaS_2.

In this work, we investigate the interplay between electronic reordering and lattice reconfiguration underlying the photoinduced transformation into a textured charge density wave and a glassy state in 1T-TaS_2. Using a combination of time-resolved diffraction and resonant and non-resonant spectroscopies, we reveal distinct in-plane and out-of-plane lattice dynamics, which accompany the electronic phase transition and ensure the longevity of the photoinduced state. Most notably, our results provide the first direct real-time observation of out-of-plane restacking and breaking of interlayer dimerization—key structural features responsible for the insulating nature of the low-temperature ground phase in 1T-TaS_2 and the main driving force behind technologically relevant ultrafast insulator-to-metal transition in the system.

We also show how these states and the associated nanoscale strains, developed in a textured system, can be leveraged for next-generation optical devices and present a novel spatial light modulator, which operates in the extreme UV and soft X-ray spectral ranges. The strain-driven electronic phase transition enables precise control of the device using coherent light beams, opening new pathways for advanced experimental techniques.

Salt Reduction and Self- Cleaning Protection of Cultural Heritage Objects by Development of New Functional Materials

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Abstract. The preservation of architectural heritage requires innovative methods that are efficient, long-lasting, and environmentally friendly. This paper presents the development of new functional materials designed for the desalination of mineral substrates and the long-term protection of inner structures through the concept of self-cleaning. The main focus of our research was design and application of two types of novel materials: clay-bio based poultices and innovative protective coating based on anionic clays. The research was implemented through six main activities, which included the development of bio-cleaning system; synthesis of anionic clay structures and the intercalation of doped nanocomposites; the establishment of assessment methods for the efficiency of the newly developed materials; their pilot production and application on cultural heritage sites (Petrovaradin Fortress, the Medieval Fortress in Arača, the Serbian Orthodox Church in Sremska Kamenica, Figure 1, the facade of the Serbian National Theatre, and the Princely Fortress in Suceava, Romania); and finally continuous monitoring using mobile equipment from the Laboratory for Materials in Cultural Heritage (HeritageLab), Faculty of Technology Novi Sad. The obtained results have demonstrated that the newly developed materials are effective not only in laboratory conditions but also in real exploitation environments, addressing key issues such as crystallization of soluble salts and persistent surface contamination in cultural heritage. The combination of clay-based desalination and bio-cleaning ensures an effective reduction of salt-induced degradation, preserving the structural integrity of historic buildings. Additionally, the application of photocatalytic self-cleaning coating (visible light driven), significantly reducing the need for frequent maintenance and minimizing the long-term impact of pollutants.

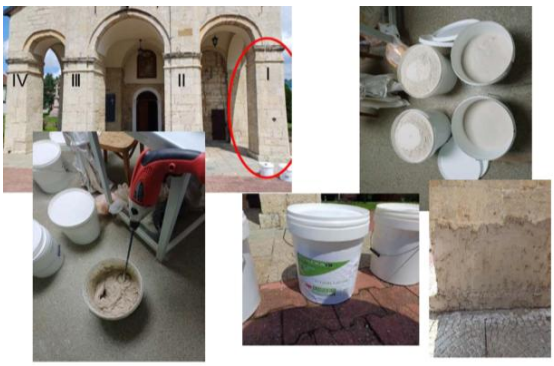

FIGURE 1. Application of newly developed bio-cleaning poultices on the Serbian Orthodox Church in Sremska Kamenica facade

Quantum Phase Transitions Above Ground States: Ergodicity Breaking Transitions

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Abstract. Quantum phase transitions in the ground states of Hamiltonian systems are rather well understood. Convenient tools for their characterisation are inspired by the quantum information theory, e.g., the entanglement entropy or the wavefunction fidelity susceptibility. For example, the peak of the ground-state fidelity susceptibility signals the quantum critical point. Here we show that quantum thermalization in isolated quantum many-body systems, along with its potential breakdowns known as ergodicity breaking transitions, share similarities with the ground state quantum phase transitions [1]. I will present an example of a quantum many-body model in which the peak of fidelity susceptibility signals the ergodicity-breaking critical point at energy densities far above ground states.

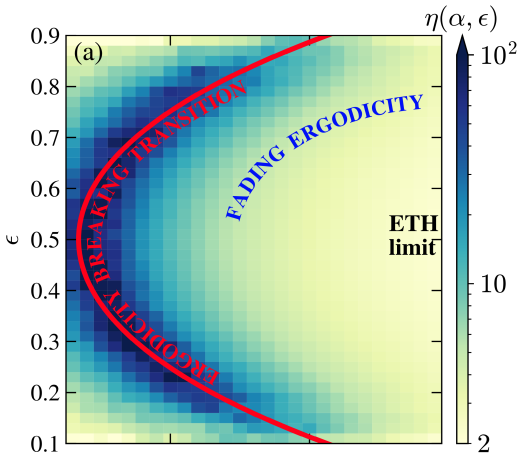

FIGURE 1. Ergodicity breaking transition at energy densities ε far above the ground state [1]. The precursor to ergodicity breaking is called *fading ergodicity* [2].

REFERENCES

1. R. Swietek, P. Lydzba and L. Vidmar, Fading ergodicity meets maximal chaos, arXiv:2502.09711
2. M. Kliczkowski, R. Swietek, M. Hopjan and L. Vidmar, Fading ergodicity, *Physical Review B* **110** 134206 (2024).

Inorganic Nanotubes and Nanowires in Polymer Matrices: Potential for Sensing Applications

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Abstract. The increasing need to move away from intrinsically rigid to flexible and wearable sensors requires finding a sensing material that responds well to mechanical deformations through a change in the electrical signal. The best way to achieve flexibility is to combine nanomaterials with polymer matrices. While the carbon nanotubes have a good potential as fillers, they have a few setbacks as well. As they do not disperse well in most organic solvents, resulting in poor homogeneity when mixed with a polymer matrix, they have to be functionalized in order to enhance the interaction with the solvent. On the other hand, various inorganic TMDC NTs promise a wide spectrum of physical effects beyond the physics of CNTs [1]. They have a high aspect ratio, high specific surface area and excellent mechanical and vibrational/acoustic properties, making them suitable as composite nanofillers as only a small amount can be used for forming a conductive path [2]. Furthermore, MS_2 NTs disperse well in all commonly used solvents, simplifying the composite preparation [3]. Another family of nanomaterials that shows a great promise as a filler, is the family of metal oxides. Their substoichiometric MO_{3-x} ($0 \leq x \leq 1$) phases grow in different shapes, such as nanowires, flakes, needles and sheets. The optical, electrical and structural properties depend strongly on the degree of the reduction [4].
Overall, these materials possess a variety of properties desirable for fabrication of sensors for human health monitoring. Despite the advancements, thorough safety assessments are needed before large-scale production and clinical deployment of nanomaterials for health sensing applications [5].

REFERENCES

1. Višić, B. et al., *JACS* **139** 12865-78 (2017)
2. Evarestov, R. et al., *Materials Research Express* ***5*** 115028 (2018)
3. Yadgarov, L. et al., Physical Chemistry Chemical Physics **20** 20812-20 (2018)
4. Višić, B., et al., Nanotechnology **33** 275705 (2022)
5. Lazarević, J. and Višić, B., under review

Towards numerically exact computation of conductivity in the thermodynamic limit of interacting lattice models

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Abstract. High temperature superconductors universally exhibit strange metallic behavior: above the critical temperature T_c, the dc resistivity is found to be a linear function of temperature, $\rho_{\mathrm{dc}} \sim T$. The T-linear resistivity is otherwise associated with quantum critical points[1], but the possible connection of this behavior with the large magnitude of the T_c is not well understood. This question is usually approached using the Hubbard model on the square lattice, yet computing the dc resistivity in this (or any other) interacting lattice model is a difficult, long-standing challenge. So far, numerically exact results have been computed only in the strong-coupling/high-temperature regime[2]. More recent results[3] indicate that in the weak-coupling regime of the Hubbard model, there is both a quantum critical point and a T-linear resistivity covering a large range of temperature. The weak-coupling results were so far computed at the level of the Boltzmann theory and at the level of the Kubo bubble. However, the respective dc resistivity results differ quantitatively, and neither theory might be exact even in the infinitesimal coupling limit. In this talk we will present our recent work[4] to develop, cross-check and apply two state-of-the-art methods for computing dynamical response functions in interacting lattice models. We compute the optical conductivity at weak coupling in the Hubbard model in a fully controlled way, in the thermodynamic limit and without analytical continuation. We show that vertex corrections persist to infinitesimal coupling, with a constant ratio to the Kubo bubble. We connect our methods with the Boltzmann theory, and show that the latter applies additional approximations, which lead to quantitatively incorrect scaling of ρ_{dc} with respect to the coupling constant. Our works opens the door to more detailed investigation of quantum critical phenomenology in the 2D Hubbard model.

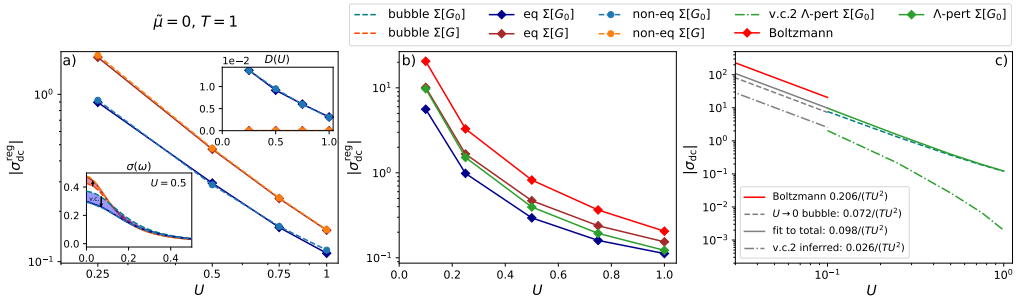

FIGURE 1. Comparison of different methods for the computation of optical and dc conductivity in the weak-coupling Hubbard model, taken from Ref.[4]

REFERENCES

1. Vučičević, J., Tanasković, D., Rozenberg, M. J., and Dobrosavljević, V. *Physical Review Letters* 114, 246402 (2015)
2. Vučičević, J. and Kokalj, J. and Žitko, R. and Wentzell, N. and Tanasković, D. and Mravlje, J., *Physical Review Letters* 123, 036601 (2019)
3. Vučičević, J., Predin, S., and Ferrero, M., *Physical Review B* 107, 155140 (2023)
4. Kovačević J., Ferrero M., and Vučičević J., *preprint*, arXiv:2501.19118 (2025)

Optimized Growth and Manipulation of Light-Matter Interaction in Stabilized Halide Perovskite Nanowire Array

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Abstract. Halide perovskite nanowires (HP-NWs) exhibit fascinating optical properties, making them attractive for advanced technologies. However, instability and lack of an effective synthetic protocol limit their commercialization. To address this, we use nanoporous anodized aluminum oxide (AAO) metamaterial as templates for the growth of perovskite ($CsPbBr_3$) NW arrays. AAO functions as both a growth template and a stabilizing medium. The NW array exhibits strong light-trapping ability, and the pore geometric features (pore radius-R and distance between pores-d) have the potential to enhance the light-matter interactions (LMI). We demonstrate the impact of R and d on LMI within the AAO/$CsPbBr_3$ system using theoretical Finite Difference Time Domain (FDTD) simulations. (Figure 1) Optimal LMI was observed with R=d=25 nm and R=d=50 nm. We report ligand-free synthesis of $CsPbBr_3$ NW arrays via spin-coating, drop-casting, and inverse temperature crystallization (ITC). The spin-coating and drop-casting yielded poor pore filling, while the modified ITC method yielded nearly complete (>90%) pore filling with significant NW lengths. Our findings highlight the potential of AAO templates for protecting $CsPbBr_3$ and addressing synthetic challenges in HPs and other semiconductor NW arrays. This study provides valuable references for LMI in HPs and advances HPs and NW array-based optical devices and renewable energy applications.

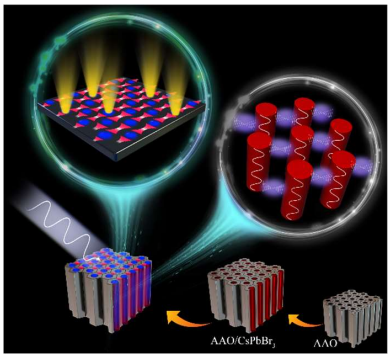

FIGURE 1. Schematic representation of the enhanced LMI and the HP's growth within the AO template.

Cell toxicity and anti-*T. gondii* efficacy of *de novo* synthesized acridine derivatives

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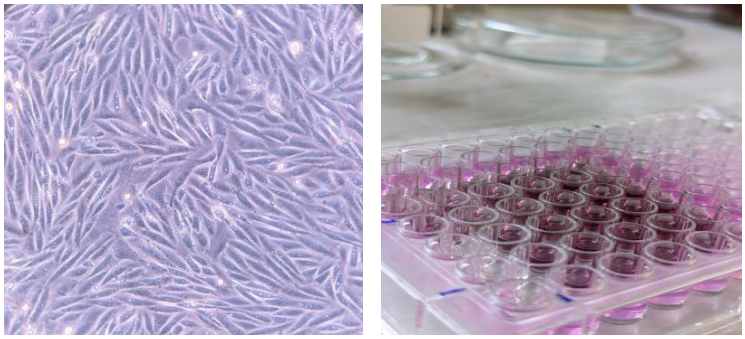
Abstract. Acridine derivatives are a group of very potent bioactive compounds with various activities such as anticancer, anti-inflammatory, antibacterial, antiparasitic and fungicidal. N-(9-acrydinil) amino acid derivatives, both previously [1] and newly synthesized were tested *in vitro* for their cytotoxicity and anti-*T. gondii* activity. *In vitro* cytotoxicity testing was performed on Vero cell line, based on MTT assay, widely used for the evaluation of cytotoxicity of newly synthesized pharmaceutical compounds. MTT assay results were displayed as CC_{50} values, obtained using GraphPad Prism 10.4.1. Anti-*T. gondii* efficacy of the synthesized derivatives was evaluated using *T.gondii* RH strain tachyzoites, by employing the trypan blue parasite viability assay after 24 hour long incubation. Results obtained so far suggest that acridine derivatives, following the structural modifications, could serve as novel drug candidates leading to more efficient and less toxic treatment options for toxoplasmosis [2]. **Acknowledgement**. This research was funded by the Science Fund of the Republic of Serbia, 7328, Reinvention of the diagnostic algorithm and treatment options for reactivated toxoplasmosis—ToxoReTREAT.



a **b**

FIGURE 1. a) Vero cells under the microscope; b) MTT assay in a 96-well plate

REFERENCES

1. Rupar, J., Dobričić, V., *et al*., *RSC Med. Chem.* 11(3), 378–386 (2020).
2. Zlatković, Đ., Dobričić, V., Srbljanović, J., *et al., Pharmaceutics 17(3), 374* (2025).

CONTRIBUTED TALKS

Electron-plasmon Scattering in Doped Graphene

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Abstract. Decay mechanisms and plasmon satellites formed in the spectrum of a photo-excited hole in doped graphene is a phenomenon that has been investigated for a long time using angle resolved photoemission spectroscopy (ARPES) measurements [1–3]. The results presented in the poster are produced by the ab initio simulation of photoemission spectra in electrostatically and chemically (KC_8) doped graphene, in the framework of our recently developed *many-body* RPA-G_0W_0 approximation. The decay width along the graphene π_+/π_- bands at the Fermi level features the exponential law $\Gamma \sim |E_{\sigma,\pi K}\text{-}E_{Fermi}|^{\alpha}$ (**Fig. 1a**), which perfectly fits the previous experimental results [1, 4], deviating from the standard Fermi liquid behavior $\alpha = 2$. At lower energies, the width of the π_+/π_- bands exhibits a peak due to the Dirac plasmon emission decay, also experimentally measured [1]. On the other hand, the plasmonic satellites appearing in the spectrum (**Fig. 1b**) feature much lower intensities than experimentally obtained [2, 3], except in the $E_{Dirac} < \omega < E_{Fermi}$ frequency range. Also, due to the Fermi liquid theory, we obtained a kink at the Fermi level in highly doped graphene (**Fig. 1b**).

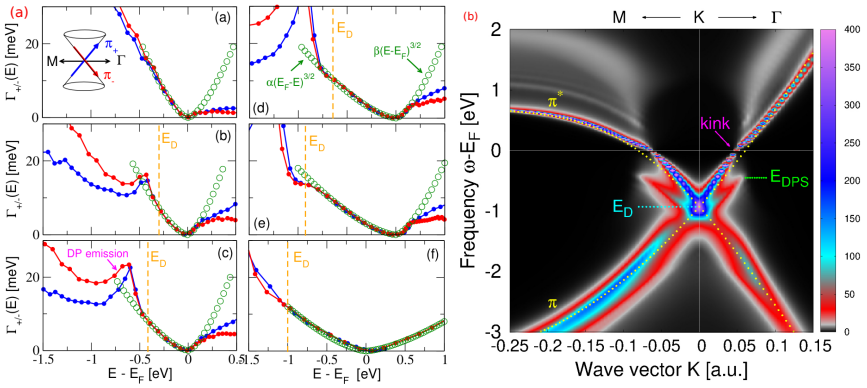

FIGURE 1. (a) The imaginary part of self-energy along π_+/π_- bands in electrostatically doped [with concentrations increasing (a)→(e)] and chemically (f) doped KC_8 graphene. (b) The simulation of spectral intensity along the high symmetry path (M←K→ Γ) in electrostatically highly doped graphene (10^{14} cm^{-2}).

REFERENCES

1. A. Bostwick, T. Ohta, T. Seyller, K. Horn and E. Rotenberg, Nature Phys. **3**, 36 (2007).
2. H. Zhang, S. Wang, E. Wang, et al, npj Quantum Mater. **6**, 83 (2021).
3. A. Bostwick, F. Speck, T. Seyller *et al*, Science **328**, 999 (2010).
4. J. Jakovac and V. Despoja, Phys. Rev. B **110**, 195425 (2024).

Unconventional temperature evolution of quantum oscillations in Sn-doped $BiSbTe_2S$ topological insulator

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Abstract. Among various topological insulators, Sn-doped Bi1.1Sb0.9Te2S stands out for its exceptional properties. It has a wide energy gap and typically exhibits a well-isolated Dirac point and a Fermi level positioned within the gap. Here, we investigate high-quality samples that display metallic-like low-temperature resistivity attributed to surface states, pronounced quantum oscillations observable even at 40 K, and a Fermi level located approximately 100 meV above the Dirac point. In this work, we focus on the quantum oscillations that show an unusual effect: a strong temperature dependence of the oscillation frequency, which decreases by around 10% between 2 and 40 K. This reduction significantly exceeds the known effects of the Sommerfeld and topological corrections for Dirac quasi-particles, which could account for only one-eighth of the observed change. We attribute the observed effect to the temperature-induced renormalization of the bulk band gap size due to electron-phonon interactions, which in turn affect the position of the surface Dirac point within the gap. Furthermore, we propose that in this compound, surface quantum oscillations can serve as a precise tool for investigating the low-temperature evolution of the bulk band gap size.

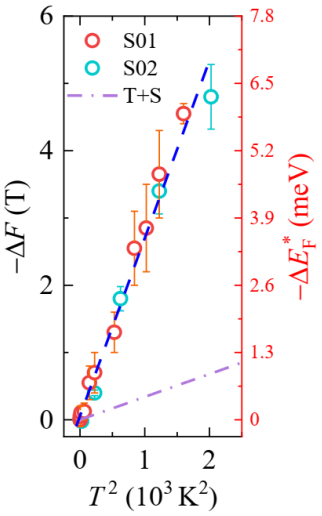

FIGURE 1. Temperature Dependence of the Quantum Oscillation Frequency Shift.

Pairing Instabilities and Critical States in Graphene Quantum Hall Systems

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Abstract. The even-denominator fractional quantum Hall effect (FQHE) in graphene, observed in the fourth Landau level ($\mathscr{N} = 3$) [1], motivates our study of pairing and ground state properties in this system. Composite fermions, formed by electrons binding magnetic flux quanta, provide a key framework for understanding FQHE in conventional systems at half-filled Landau levels. Using the dipole representation of composite fermions [2], we derive an effective Hamiltonian for half-filled Landau levels, emphasizing particle-hole symmetry. At the Fermi level, the interplay of topology and symmetry drives the system toward a critical state. While we explore the possibility of paired states with well-defined solutions, our results show that the energetically favored state is a regularized, boost-invariant configuration without pairing instabilities [3]. This finding holds for the half-filled fourth Landau level ($\mathscr{N} = 3$) in graphene. We discuss the consistency of our results with experiments and simulations, highlighting the need for further research into alternative configurations in quantum Hall systems.

REFERENCES

1. Y. Kim, A. C. Balram, T. Taniguchi, K. Watanabe, J. K. Jain, and J. H. Smet, *Even denominator fractional quantum Hall states in higher Landau levels of graphene*, Nature Phys. **15**, 154 (2019).
2. S. Predin, A. Knežević, and M. V. Milovanović, *Dipole representation of half-filled Landau level*, Phys. Rev. B **107**, 155132 (2023).
3. Sonja Predin, *Dipole representation of composite fermions in graphene quantum Hall systems*, Phys. Rev. B **111**, 045132 (2025).

Coherent Phonon Raman Spectroscopy as an Emerging Technique for Space Exploration

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Abstract. Raman spectroscopy is a suitable method for identifying minerals and their compositions for in-situ planetary research. Development of space-ready femtosecond lasers [1, 2] enable alternative approaches, time-domain techniques. Time-domain techniques have the advantage of being compact and chip-integrable. We investigate the potential of coherent phonon spectroscopy (CPS) as an alternative to Raman-spectroscopy [3]. The applicability of CPS as an in-situ technique to identify matter by their characteristic spectra of Raman-active phonons is evaluated. We show that a spectral bandwidth of beyond 30THz (~ 1000cm^{-1}) and a resolution of 100 GHz (~ 4cm^{-1}) can be achieved, while any fluorescence background is avoided.

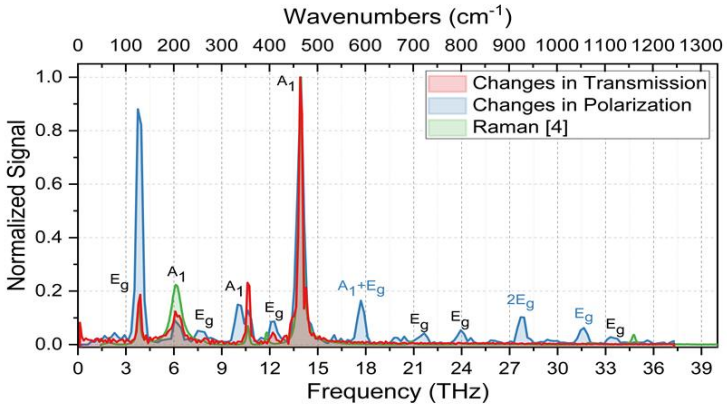

FIGURE 1. Raman spectrum of Quartz taken from the RRUFF database [4] and CPS spectra. All expected Raman-active modes are observed. The polarization-sensitive CPS reveals additional expected (combination) modes.

REFERENCES

1. J. Lee, et al, *Scientific Reports* (2014); **4**, 5134.
2. M. Lezius et al, *Optica* (2016); **3**, 1381
3. Ishioka, K., Misochko, O.V. Coherent Lattice Oscillations in Solids and Their Optical Control. In: Progress in Ultrafast Intense Laser Science. *Springer Series in Chemical Physics*, vol **98**. (2010).
4. B. Downs, Quartz R040031, *rruff.info*. https://rruff.info/Quartz/R040031

POSTER SESSION

Predicting Polymer–Drug Interactions Using Hansen Solubility Parameters: A Study on SSRIs

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Abstract. Polymers have become a helpful tool in improving drug delivery systems by allowing medications to be released in a controlled way over time. This helps in providing a steady dose of both hydrophilic and hydrophobic drugs, which can increase their effectiveness and reduce the need for frequent doses [1]. In this study, we focus on selective serotonin reuptake inhibitors (SSRIs) fluoxetine and sertraline. Even though these drugs are commonly used, their interactions with polymers have not been investigated. The main goal of this research is to look into how polymers can bind with these SSRIs, which might help improve solubility, control release, and bioavailability, while also reducing side effects. In parallel, these assessments may also help in studying the polymers and potential filters for pharmaceuticals in the environment.

To achieve this, we use Hansen solubility parameters (HSPs) as a tool to predict how well polymers and drugs will interact. HSPs measure how substances interact through dispersion, polarity, and hydrogen bonding forces [2], which can help us choose the best polymers for further experimental testing. Preliminary findings indicate that polyethylene oxide, polysulfone, poly(methacrylic acid) are the most compatible out of the selected polymers with target drugs based on the HSP Distance between two molecules *(Ra),* interaction radius *(R0)* and Relative Energy Difference (*RED)* values *(RED*<1).

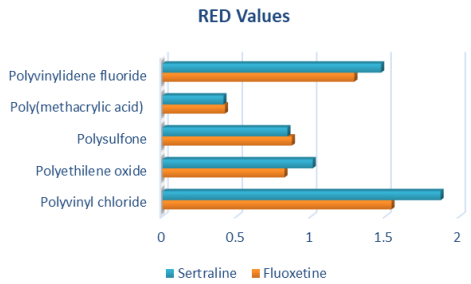

FIGURE 1. Chart showing RED values of the selected polymers

REFERENCES

1. Liechty, W., Kryscio, D., Slaughter, B., Peppas N. Annu Rev Chem Biomol Eng. 2010, **1**, 149-73.
2. Hansen, C. M. In: Hansen Solubility Parameters: A User's Handbook, Second Edition, CRC Press, 2007, 4.

Effects of Exfoliation Parameters and Relative Humidity on the Structure of Kaolinite Nanoplates

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Abstract. We investigated the influence of exfoliation parameters and exposure to relative humidity (RH) on the inner and external hydroxyl groups of kaolinite nanoplates obtained by liquid-phase exfoliation (LPE) and deposited onto the solid substrate using the Langmuir-Blodgett technique. Kaolinite, a naturally occurring layered aluminosilicate, is widely used in nanocomposites, environmental remediation, and biomedical applications [1]. Its hydroxyl-rich surface readily interacts with water molecules, particularly under varying humidity, thereby altering its physicochemical properties. While the exfoliation increases the surface area, introduces defects, exposes inner layers and may lead to reorientation or partial removal of hydroxyl groups, high RH conditions can affect the surface hydroxylation by promoting H-bonding, as well as the regeneration and rearrangement of hydroxyl groups [2, 3]. In our study, we demonstrate how both LPE parameters (water content of the solvent, exfoliation time, and the initial concentration of bulk material), and exposure to high RH (>70%) affected the structure of produced kaolinite nanoplates. UV-VIS spectroscopy, XRD, Raman Spectroscopy and AFM confirmed the successful exfoliation of the material, while FTIR indicated that exfoliation conditions could be effectively tuned to control and optimize the hygroscopic behavior of kaolinite nanoplates.

This research was supported by the Science Fund of the Republic of Serbia, Grant No 7456, 2D Material-based Tiled Network Films for Heritage Protection-2DHeriPro.

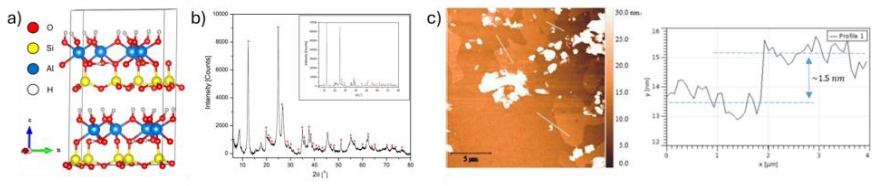

FIGURE 1. a) Crystal structure of kaolinite, b) XRD patterns of LPE and bulk kaolinite (inset), c) AFM image of kaolinite nanoplates (left) with height profile (right).

REFERENCES

1. Nisticò, R. Inorganics **10**, 40 (2022).
2. X. Huang et al., Langmuir **35** 13833–13843 (2019).
3. Kloprogge, J., Spectroscopic Methods in the Study of Kaolin Minerals and Their Modifications, Springer Mineralogy, Springer, Cham., 2019, pp. 41-96

Raman Signatures Of Instabilities In $InSiTe_3$

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Abstract. Layered van der Waals materials have gained considerable interest for their unique physical properties, yet $InSiTe_3$ remains largely unexplored due to uncertainties surrounding its crystal structure. In this work, we present a comprehensive experimental and theoretical investigation of $InSiTe_3$, confirming a rhombohedral structure with $P\bar{3}$ space group symmetry via single-crystal X-ray diffraction. Polarization-resolved Raman scattering reveals nine out of ten Raman-active modes expected for this symmetry, further validating the structural assignment. Beyond conventional phonon behavior, we identify strong anharmonicity and the emergence of a self-organized coherent phonon state associated with a high-energy A_g mode near 500 cm^{-1}. Analysis of phonon-phonon coupling parameters indicates that A_g modes exhibit coupling strengths up to eight times greater than E_g modes. Temperature-dependent Raman measurements from 80 to 300 K reveal notable changes in A_g mode intensities around 200 K and the appearance of broad spectral features in the phonon gap region, attributed to overtone excitations. Our findings point to an intrinsic lattice instability in $InSiTe_3$, driven by strong anharmonic interactions. However, further studies are required to fully uncover the microscopic origin of these instabilities and their implications for the material's physical properties.

*This research was supported by the Science Fund of the Republic of Serbia, 10925, Dynamics of CDW transition in strained quasi-1D systems – DYNAMIQS

Raman Spectroscopy Analysis Of Disorder Effects In *2H*-$TaSe_{2-x}S_x$ Alloys

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Abstract. Layered transition metal dichalcogenides (TMDs) possess remarkable electronic and optical properties, largely due to their quasi-two-dimensional structures. These materials display complex phase diagrams and temperature-driven transitions [1]. In these compounds charge density wave (CDW) and superconductivity (SC) are shown to coexist at certain temperatures - illustrating the delicate balance and inherent competition between these two phases [2]. Isoelectronic substitution such as sulfur doping in *2H*-$TaSe_{2-x}S_x$, primarily introduces disorder, which disrupts the CDW phase and enhances superconductivity [3]. Tuning properties through doping and structural changes highlights the potential of TMDs for future quantum materials and devices.

In this work, we examined the lattice dynamics of *2H*-$TaSe_{2-x}S_x$ single crystals ($0 \leq x \leq 2$) using Raman spectroscopy alongside density functional theory (DFT) calculations. For the undoped samples, the Raman spectra show two out of the four symmetry-allowed modes and a broad two-phonon feature, which is correlated with strong electron–phonon coupling (EPC). With sulfur doping, the induced disorder opens new scattering channels, giving rise to extra peaks. Our results indicate that disorder minimally affects the EPC, suggesting that while the CDW phase is sensitive to structural changes, the SC state remains robust. Overall, our study sheds light on how crystallographic disorder and EPC shape the Raman response and lattice dynamics in these compounds.

REFERENCES

1. Wang, Q. et al. Electronics and optoelectronics of two-dimensional transition metal dichalcogenides. *Nature Nanotech* **7**, 699–712 (2012).
2. F. Zheng and J. Feng, Electron-phonon coupling and the coexistence of superconductivity and charge-density wave in monolayer $NbSe_2$, *Phys. Rev. B* 99, 161119 (2019).
3. L. Li et al, Superconducting order from disorder in *2H*-$TaSe_{2-x}S_x$, npj Quantum Materials 2 (2017).

OQCET: Open Quantum Cluster Embedding Theory

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Abstract. We introduce the open quantum cluster embedding theory (OQCET), an embedded cluster method aimed at computing the response of the system following an external perturbation. [1] This allows one to reconstruct dynamical susceptibilities in the manner of inverse linear response theory. The method is feasible for very large lattices and avoids analytical continuation. OQCET becomes numerically exact in the infinite cluster size and the non-interacting limits, and it respects total charge and energy conservation laws. The embedded clusters are open quantum systems governed by the Lindblad equation. Short-range correlations extracted from the clusters are used on the lattice to close the equations of motion for the fermionic bilinear and the local double occupancy. We apply the method in computation of the charge-charge and current-current correlation functions in the square lattice Hubbard model and analyze the results.

REFERENCES

1. Petar Brinić, Hugo U. R. Strand and Jakša Vučičević, in preparation.

A Study Of Oxidized MoS_2

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Abstract. Two-dimensional (2D) semiconductors, such as molybdenum disulfide (MoS_2) exhibit electronic and optical properties suitable for various applications in *e.g.*: nanoelectronics, sensors, and photonics [1]. Thermal annealing, likely to trigger oxidation processes, is commonly used during the fabrication of devices, either to eliminate contaminants or to modify their electronic characteristics [2].
In order to elucidate the role of number of layers and oxidation on the behavior of exfoliated MoS_2 flakes, a comprehensive study of second harmonic generation (SHG) and Raman spectroscopy, has been carried out on a series of flakes with thickness in the range from one to nine layers. Furthermore, polarization dependent SHG is used for revealing the underlying crystalline structure of the systems. The oxidation process is controlled using a rapid thermal annealer, where the duration is adjusted while keeping the temperature fixed at 300°C with a constant oxygen flow. Especially for the flakes with an even number of layers, oxidation allows establishing the hexagonal structure in the polarized SHG, which hints at a layer-by-layer oxidation with the here used parameters. The results provide insights into the oxidation process in atomically thin MoS_2 and highlight the relevance of the number of layers in determining the stability and efficiency of MoS_2-based devices.

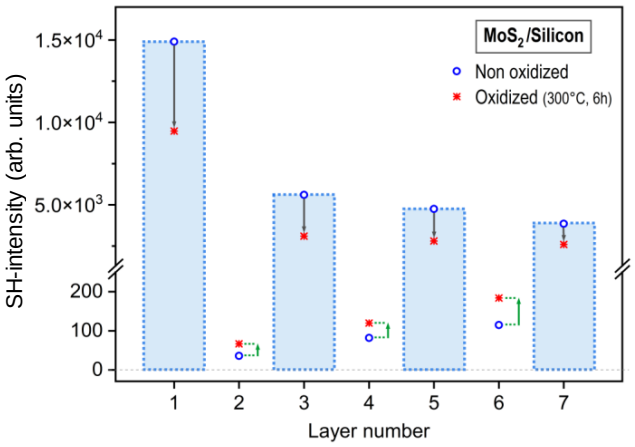

FIGURE 1. SH-Intensity as a function of number of layers for non-treated and for 6h oxidized MoS_2.

REFERENCES

1. M. Wang *et al*., *Nat. Electron* **1**, 130 (2018)
2. Y. Jiang, *et al*., *Nanotechnol.*, **34**(40), 405701 (2023)

Precise Control of Structure and Magnetic Properties of $BiFeO_3$: From Synthesis to Prediction of New Modifications

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Abstract. In recent years multiferroics have been an intriguing study field due to their well-known magnetoelectric phenomena that offer a wide range of potentially new applications including spintronics, new data storage media and multiple-state memories [1–5]. Bismuth ferrite (BFO) particles were synthesized via a controlled hydrothermal method, yielding highly pure, small-sized particles. Structural characterization revealed that the as-synthesized (non-annealed) powder crystallizes in the rhombohedral R3c space group with minimal secondary phase content. Upon annealing at 800 °C, a single-phase perovskite structure with high crystallinity was obtained. High-resolution transmission electron microscopy (HRTEM) analysis confirmed the presence of twin stacking faults, which are responsible for enhanced magnetic properties. Electron paramagnetic resonance (EPR) spectroscopy measurements suggested the existence of electrons trapped by vacancies or defects. It has been proposed that the existence of Fe^{3+}–O_V defect complex could be generated at elevated temperatures followed by the formation of trivalent Fe ions, which intensely provide local 3d moments. In addition, a structure prediction has been performed and 11 additional $BiFeO_3$ modifications have been proposed, while the magnetic behavior of synthesized material was investigated by SQUID.

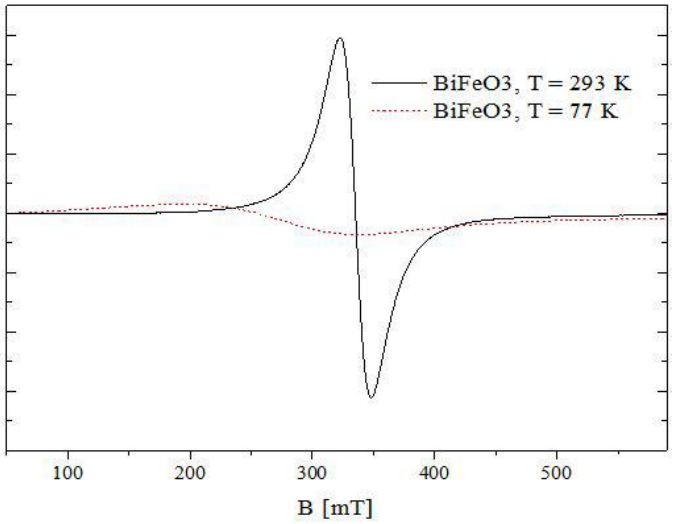

FIGURE 1. EPR spectra of the BFO powder measured at T = 293 K and T = 77 K

REFERENCES

[1] Martin, L. W., Crane, S. P., Chu, Y. H., Holcomb, M. B., Gajek, M., Huijben, M., Yang, C. H., Balke, N., Ramesh, R., *J. Phys.: Condens. Matter*, **20**, 434220–434233 (2008).
[2] Catalan, G., Scott, J.F., *Adv. Mater.* **21**, 2463–2485 (2009).
[3] Rojac, T., Bencan, A., Malic, B., Tutuncu, G., Jones, J.L., Daniels, J.E., Damjanovic, D., *J. Am. Ceram. Soc.* **97**, 1993–2011 (2014).
[4] Wang, J., Neaton, J.B., Zheng, H., Nagarajan, V., Ogale, S.B., Liu, B., Viehland, D., Vaithyanathan, V., Schlom, D.G., Waghmare, U.V., Spaldin, N.A., Rabe, K.M., Wuttig, M., Ramesh, R., *Science* **299**, 1719–1722 (2003).
[5] Teague, J.R., Gerson, R., James, W.J., *Solid State Commun.* **8**, 1073–1074 (1970).

Spin-Lattice Coupling and Multiferroic Modulation in Ho-Doped $BiFeO_3$: An Experimental and Theoretical Study

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Abstract. Bismuth ferrite ($BiFeO_3$, BFO) is one of the most intensively studied multiferroic materials due to its simultaneous ferroelectric and antiferromagnetic behaviour at room temperature, making it highly promising for a wide range of technological applications, including spintronics, memory devices, and sensor technologies [1-3]. Despite significant research interest, controlled tuning of its electronic and magnetic properties through rare-earth doping remains a fundamental and practical challenge. We systematically investigated the effects of Ho doping on the structural, electronic, and magnetic properties of BFO using a combined experimental and theoretical approach. Nanopowders with the composition $Bi_{1-x}Ho_xFeO_3$ ($x = 0.02, 0.05$, and 0.10) were synthesized by hydrothermal synthesis, and their crystal structure was thoroughly analyzed using X-ray diffraction (XRD), revealing phase stability with gradual structural transformations dependent on dopant concentration.

Furthermore, bond valence calculations (BVC) identified six energetically favourable structural modifications of the Ho-doped system: a-, b-, g-, R-, T_1-, and T_2-phases. These structural configurations were further examined using advanced computational simulations based on density functional theory (DFT) to evaluate the stability of different magnetic orderings, electronic structures, and the evolution of ferroelectric properties with increasing Ho concentration.

The results of our theoretical and experimental investigations reveal a rich spectrum of electronic and magnetic phenomena in Ho-doped BFO, offering new insights into the control of multiferroicity through doping. These findings have significant implications for further research and the development of advanced multiferroic materials with enhanced functional properties, suitable for innovative nanoelectronics and spintronic applications.

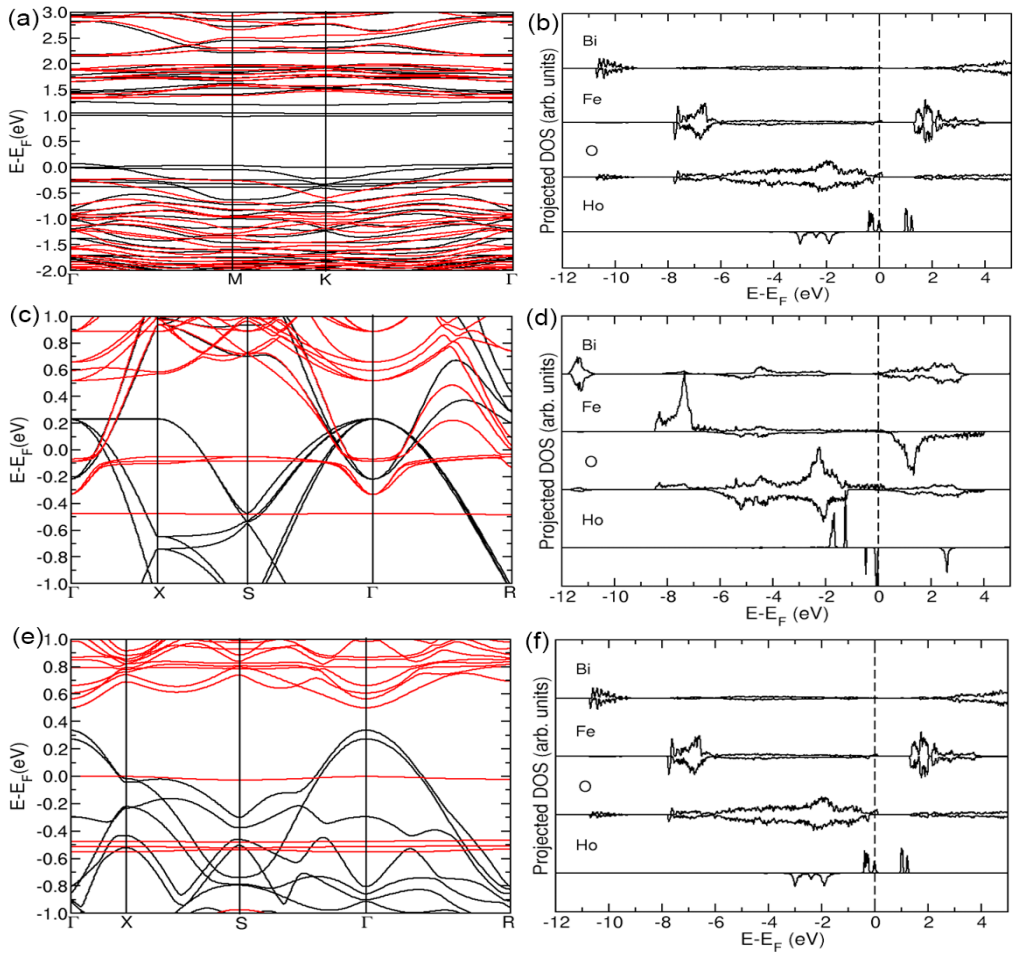

FIGURE 1. Electronic band structure of alpha AFM1 (a), gamma FM (c), T1 FM (e) and elements-resolved density of states of alpha AFM1 (b), gamma FM (d) and T1 FM (f) phases. Black lines present spin-up and red lines spin-down bands. Mirrored graphs of the density of states correspond to spin-up and spin-down states.

1. Rödel J. , Jo W., Seifert K.T.P., Anton E.-M., Granzow T., Damjanovic D., "Perspective on the development of lead-free piezoceramics", J. Am. Ceram. Soc., **92** 1153–1177 (2009).
2. Fruth V., Mitoseriu L., Berger D., Ianculescu A., Matei C., Preda S., Zaharescu M., "Preparation and characterization of $BiFeO_3$ ceramic", Progress Solid State Chem., **35** 193–202 (2007).
3. Liu K., Fan H., Ren P., Yang C., "Structural, electronic and optical properties of BiFeO3 studied by first-principles", J. Alloys Comp., **509** 1901– 1095 (2011).

The Electronic Structure of Ag-Bi-S-I Nanomaterials Studied by X-ray Aerosol Photoelectron Spectroscopy

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Abstract. Silver-Bismuth iodide rudorffites emerged as promising lead-free, non-toxic, and chemically stable materials for photovoltaic applications. Recently, we developed two novel synthesis routes to obtain Ag-Bi-I nanoparticles [1, 2]. Motivated by a recent study that demonstrated that partial substitution of I^- with S^{2-} ions can lead to band gap modification due to upshifting the valence band maximum in the presence of sulfide anions, thereby enhancing photoconversion efficiency in solar cells, we also synthesized Ag-Bi-S-I and $AgBiS_2$ nanoparticles. We performed synchrotron radiation X-ray aerosol photoelectron spectroscopy (XASP) to study the difference in the valence electronic structure of Ag-Bi-I, $AgBiS_2$, and Ag-Bi-S-I nanoparticles. This technique allows for the analysis of isolated nanoparticles free from solvent and ligand molecules [4, 5]. Additionally, the use of tunable synchrotron radiation wavelengths enables the acquisition of high-resolution spectra from highly diluted systems.

REFERENCES

1. Danilović, D., Božanić, D. K., Dojčilović, R…, *J. Phys. Chem. C* **124**, 23930-23937 (2020).
2. Danilović, D., Milosavljević, A. R., Sapkota, P..., *J. Phys. Chem. C* **126,** 13739-13747 (2022).
3. Danilović, D., Nahon, L., Garcia, G. A..., *ChemPhysChem*, ***25***, e202400328 (2024).
4. Danilović, D., Božanić, D. K., Garcia, G. A..., *Opt. Quantum Electron.* ***54***, 604 (2022).

Obtaining activated carbon materials from almond and walnut shells and their application

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This work investigates the potential of carbon materials derived from biowaste, specifically almond and walnut shells, as sustainable sources of carbon materials for various applications, such as energy devices, filtration and energy storage. Almond and walnut shells, rich in organic matter, are subjected to pyrolysis processes to obtain highly porous carbon materials with specific characteristics required for industrial applications. In this research, parameters such as pyrolysis temperature, treatment time, porosity and electrical conductivity of the obtained carbon materials were analyzed. The results showed that carbon materials derived from almond and walnut shells have significant potential for applications in the field of energy efficiency and environmental protection, due to their high surface activity and porous structure.

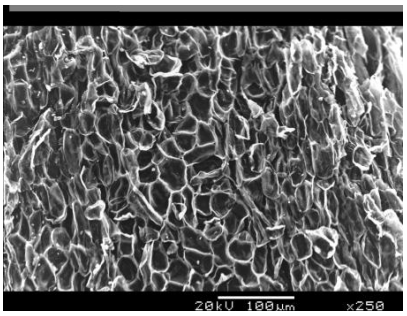

FIGURE 1. Activated carbon material obtained from almond shells at 850°C

REFERENCES

1. Bhat, M. I., et al. "Biochar from almond and walnut shells as an effective material for adsorption of heavy metals." *Journal of Environmental Management*, **275**, 111301 (2020).

2. Lee, J., et al. "Sustainable carbon materials derived from agricultural waste for energy and environmental applications." *Energy and Environmental Science*, **14**(4), 1456-1467 (2021).

Exploring Electrical and Optical Properties: 2D GaS 1T vs 2H

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Abstract. Two dimensional materials offer unique electronic, optical and mechanical properties, making them ideal candidates for next-generation technologies in electronics, energy storage and light sensing technologies. The newest addition to transitional metal dichalkogenides-gallium sulfide (GaS) [1], in its monolayer form has shown notable electronic and optoelectronic properties.

In its monolayer form, GaS adopts a hexagonal structure and exists in two phases (2H and 1T). Both phases possess a wide band gap, highlighting their potential for optoelectronic applications. This study focuses on electronic and optical properties of both phases, as well as the investigation of the solid-solid phase transition [2] between them.

Our research examines the crystal structure, electrical and optical properties of these phases. The calculations were performed using the Quantum ESPRESSO software package [3], based on density functional theory, plane waves and pseudopotentials.

The results of this study contribute to advancements in phase-switching applications, highlighting GaS as a novel, stable, and non-toxic material with excellent performance in the UV range.

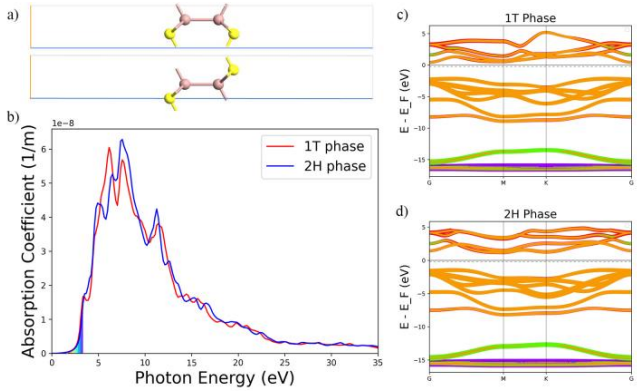

FIGURE 1. a) Structure of the two phases of monolayer GaS, the 2H phase (up) and 1T phase (down); b) Graph showing the absorption coefficient of the two phases; (c,d) band structure of the two phases

REFERENCES

1. Chen,H et al. , RSC Adv.5, 50883-50889, (2015)
2. Zhou et al, Chemistry Select, 1, 5779-5783 (2016)
3. Giannozzi P et al. J Phys Condens Matter, 30;21(39):395502 (2009)

Beyond Perfection: Lattice Defects and Light Manipulation in Diatom Frustules

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Abstract. Diatom frustules, with their periodic nanostructures, function as natural 2D photonic crystals, making them valuable for biosensing and bio-optical applications [1]. While their highly ordered pore patterns influence light propagation, real-world specimens exhibit inherent lattice imperfections that can alter their photonic behavior. In this study, we explore the impact of grid size variations, structural defects, and irregularities on the guided mode resonance (GMR) in Aulacoseira spp. frustules. Using COMSOL Multiphysics simulations we analyze how blocked pores, duplicated pores, and variations in frustule diameter affect light interactions. Our results reveal that lattice irregularities can enhance GMR, accompanied by a redshift effect, suggesting that imperfections may play a functional role in tuning optical responses. These insights provide a deeper understanding of the interplay between structural defects and photonic behavior in diatoms, opening new possibilities for biomimetic photonic materials and applications in optical sensing.

REFERENCES

1. Gilic, M., Ghobara, M., and Reissig, L., *Nanomaterials* **13**, 1594-1605 (2023).

Decoding the Pigments of the Past: Raman Spectroscopy on Historical Banknotes

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Abstract. Banknotes represent a complex material particularly suitable for analysis using Raman spectroscopy, primarily due to their dimensions, which allow examination using sophisticated laboratory instruments without requiring instrument mobility. Comparing pigments on the same or different banknotes, identifying natural and synthetic pigments from various historical periods or manufacturers, provides insight into the technological evolution and production of pigments and banknotes, international cooperation and trade, as well as the authenticity of the banknotes themselves [1]. A total of 53 banknotes from the period between 1893 and 2018, used in the territory of present-day Serbia, were examined. The identified pigments were documented and their presence on the analyzed historical banknotes was mapped over time. The temporal distribution of detected pigments aligns with the emergence, use, and mass production of synthetic pigments, which began in the 19th century and continued into the first half of the 20th century [2,3]. In addition to extensive historical and archival materials, printing techniques were studied with a particular focus on security printing processes in order to determine factors significant for monetary culture and banknote protection in Serbia [1].

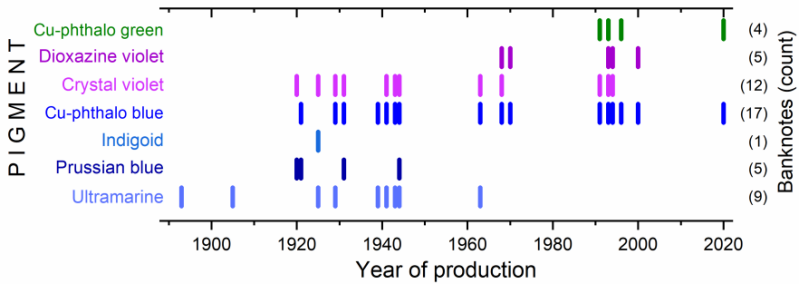

FIGURE 1. The temporal distribution of blue, purple, and green pigments used in banknote production.

REFERENCES

1. G. Jauković, Formation and Historical Development of Visual Identity in Service of Protection of Coins and Banknotes in Serbia (1868-2018) (PhD thesis, University in Belgrade, Studies at the University Multidisciplinary Postgraduate Studies, 2021).
2. M.C. Caggiani, A. Cosentino, A. Mangone, Microchemical Journal 129 (2016) 123–132.
3. W. Fremout, S. Saverwyns, J. Raman Spectrosc. 43 (2012) 1536-1544.

Temperature and shape dependent band gap for halide perovskite nanocrystals

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Abstract.

In spite of great progress, that started with the development of efficient perovskite solar cell (PCE) in 2012, when power conversion efficiency of 10.9% was achieved [1], there are much concerning issues, like longevity and special disposal of these materials, due to the presence of highly toxic Pb atoms. Even though it is possible to replace or greatly reduce the presence of Pb atoms, devices based on such materials have shown significantly inferior stability and performance compared to their Pb-based variants. Nevertheless, there is much to be learned by studying Pb-based halide perovskites which can help us to better understand these types of materials in order to improve their performance and even provide an insight on how to match this performance with Pb-free variants.

In order to give reliable and accurate theoretical predictions on performance and stability of halide perovskite nanocrystals, one should first obtain a good knowledge about their bulk electronic structure. Conventional DFT yields accurate band gaps due to the cancellation of errors when using local or semi-local functional and neglecting spin-orbit coupling (SOC) effects. However, even with hybrid functional and SOC treatment, the prediction for halide perovskite band gap cannot capture the temperature dependent influence of electron-phonon interaction which significantly opens the band gap. Only once a proper value of the band gap w.r.t. the experiment is obtained, can one proceed to give predictions for nanostructures.

In order to produce a reliable band gap, we propose the use of DFT with hybrid PBE0 functional, combined with Allen-Heine-Cardona (AHC) theory and the evaluation of anharmonic phonon frequencies using self-consistent phonon method [2]. Furthermore, we proposed a procedure, based on the self-consistent Migdal approximation, to evaluate the electronic spectral functions. This way, our procedure accounts for energy level renormalization and broadening at the same time by obtaining them self-consistently. We obtain $CsPbX_3$ (X=Cl, Br, I) band gaps for a wide range of temperatures and compare them with available experimental data.

Next, we use the obtained electronic structure to construct symmetry-adapted $\mathbf{k}\cdot\mathbf{p}$ Hamiltonians using the method what we developed in Ref. [3]. Using these Hamiltonians we obtain band gaps for $CsPbX_3$ quantum wells, wires and dots of sizes between 2 nm and 12 nm and temperatures ranging from 300 K to 700 K.

REFERENCES

1. M. M. Lee, J. Teuscher, T. Miyasaka, T. N. Murakami and H. J. Snaith, *Science*, **338**, 643–647 (2012).
2. Jocić, M., Vukmirović, N., *Phys. Chem. Chem. Phys.* **25**, 29017 (2023).
3. Jocić, M., Vukmirović, N., *Phys. Rev. B* **102**, 085121 (2020).

Structural and Electronic Properties of Y_2O_2S: A Theoretical Assessment and Predictions

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Abstract. Yttrium oxysulfide (Y_2O_2S) is a compound of significant interest due to its wide range of industrial applications, including its use as a luminescent material. In short, yttrium oxysulfide is best known for its use in light sources and phosphors, but it is also used in science and technology where specific luminescent properties are needed. This study investigates the energy landscape and electronic properties of Y_2O_2S using crystal structure prediction and first-principles calculations. The structural and electronic properties of Y_2O_2S are analyzed through Density Functional Theory (DFT), employing various functional such as Local Density Approximation (LDA), Generalized Gradient Approximation (GGA), and the hybrid B3LYP functional. Global optimization techniques were applied to explore potential new crystal structures, identifying three unique modifications: alpha, beta, and gamma. These structures were subsequently optimized and analyzed for stability and electronic properties, including the calculation of the band gaps and density of states (DOS). The alpha-type structure was found to have a band gap of approximately 4.73 eV, consistent with previous theoretical results [1]. Meanwhile, the beta-type modification showed a larger band gap of 6.26 eV, which is in agreement with prior findings [2]. The study provides a comprehensive overview of the electronic structure of Y_2O_2S, highlighting its potential for use in luminescent and semiconductor applications, and offers new insights into its energy landscape that could guide future material design and optimization.

REFERENCES

1. Chen, X., Zhang, L., & Wang, Y., "Theoretical study of the electronic structure of yttrium oxysulfide Y_2O_2S", *Journal of Materials Science*, (2014), 49(9), 3146-3152.
2. Li, S., Xu, Z., & Zhang, Y., "Electronic properties of yttrium oxysulfide and its potential applications", *Journal of Applied Physics*, (2012), 111(5), 056105

DFT Study of Glutamine (L) Interactions with Pristine and Au / Ag / Cu Doped TiO_2 Surfaces: Energy Landscape and Potential Biomedical Applications

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Abstract. This study connects inorganic and organic systems through a theoretical investigation of the energy landscape of a molecule–substrate interaction, focusing on glutamine (L) adsorbed on pristine and doped TiO_2 crystal modification, anatase, in a vacuum. We explored potential inorganic–organic interactions within these systems, depending on the properties of the TiO_2 material under investigation, which may have applications as a possible anticancer agent or nanoscale therapeutic. Glutamine was selected as the model molecule due to its important role in cancer metabolism—it serves as an alternative to glucose for fueling the tricarboxylic acid (TCA) cycle in cancer cells, with many tumor cells relying on extracellular glutamine for survival [1,2]. To simulate the interactions between nanoparticles and an amino acid molecule, we constructed systems with different glutamine conformations onto quasi-2D slab surfaces of anatase TiO_2, oriented along the (001) and (101) planes, both in their pristine form and doped with Au, Ag, or Cu. Ab initio calculations were performed using Density Functional Theory (DFT) with the LDA and GGA-PBE functionals, employing two different computational codes—CRYSTAL17 and Quantum Espresso [3]. Given the low symmetry and high atomic complexity of these systems, the calculations were computationally intensive and required substantial memory resources. To optimize the search for low-energy configurations of molecule on ceramic-type surfaces, we implemented an iterative approach that alternated between doped and undoped surfaces, which proved to be highly efficient for identifying stable structures in inorganic–organic systems of this nature. The most important result of this study might be that even without exposing the system to high temperatures or irradiation by high-energy photons, we find that just the simple adsorption process of glutamine on TiO2 surfaces can locally release enough energy to lead to a break-up of the molecule. Furthermore, by selecting different types of doping of the anatase substrate and varying the initial orientation of the molecule, this nanocrystalline material can be used for fine-tuning the physical and chemical interactions with the glutamine molecule or inducing a break-up of, or a dissociation of H atoms from the molecule (Figure 1), which provides important insights for future research and potential applications in biomedicine [3].

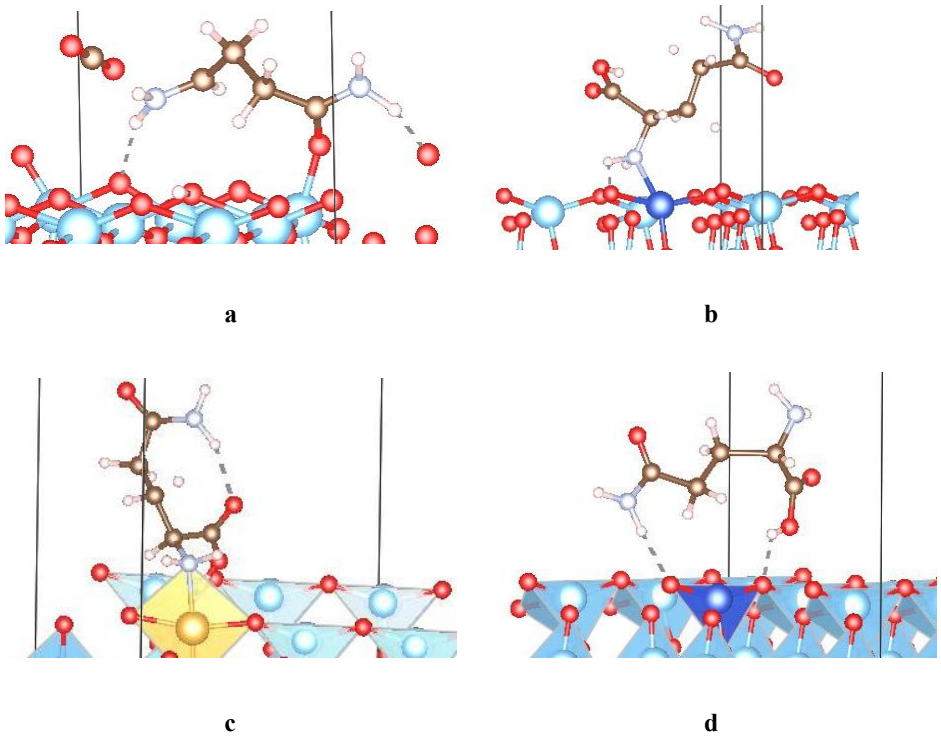

FIGURE 1. Presentation of dominant interactions in this study between (metal atoms in) the various undoped and doped anatase slab surfaces (a (001), and b–d (101) surface orientation) and molecule's: a) amino, amide, and carboxyl groups, with specific denaturation of carboxyl group—linear chain; b) direct interaction with dopant atom and separation of hydrogen atoms of the molecule; c) round-like shape deformation of molecule and separation of hydrogen atoms, and d) heart-shaped deformation of the molecule, with carboxyl and amide group interactions (visualized by Vesta program) [3].

REFERENCES

1. Corbet, C., and Feron, O., *Curr. Opin. Clin. Nutr. Metab. Care* **18**, 346–353 (2015).
2. DeBerardinis, R.J., Lum, J.J., Hatzivassiliou, G., and Thompson, C.B., *Cell Metab.* **7**, 11–20 (2008).
3. Jovanović, D., Schön, J.C., Zagorac, D., Zarubica, A., Matović, B., and Zagorac, J., *Nanomaterials* **13**, 2688 (2023).

Symmetry-Resolved Raman Study of Temperature-Induced Phonon Anomalies in $ZrTe_5$

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Abstract. Zirconium pentatelluride ($ZrTe_5$) has attracted considerable attention in the condensed matter community due to its temperature-dependent band gap variations. Additionally, it has been proposed that $ZrTe_5$ lies near a phase boundary between strong (STI) and weak topological insulator (WTI) phases, as well as undergoing an electronic topological (Lifshitz) transition. Depending on the sample and synthesis conditions, the Lifshitz transition temperature varies between 50 and 150 K [1–3]. In this study, we performed Raman spectroscopic analysis of $ZrTe_5$ single crystals over a temperature range of 76 to 300 K. The measurements were carried out in symmetry-resolved scattering geometries using parallel and cross polarization configurations along the principal crystallographic directions. In this setup, only phonon modes of A_g and B_{2g} symmetries are allowed in the respective configurations. The results reveal pronounced temperature-dependent behavior, including variations in phonon linewidths and peak positions. Notably, at lower temperatures, certain phonon modes exhibit asymmetric line shapes that are well described by the Fano profile. As the temperature increases, these features gradually evolve into symmetric peaks. This behavior indicates a strong coupling between lattice vibrations and electronic excitations in $ZrTe_5$. Our Raman scattering results provide valuable insight into the phonon dynamics and electron–phonon coupling in $ZrTe_5$, contributing to a deeper understanding of its fundamental properties.

REFERENCES

1. Zhang, J., Wang, C., Wang, J., et al. “Signatures of a Lifshitz Transition in the Mixed Dirac-Weyl Semimetal $ZrTe_5$,” Phys. Rev. B 108, L041202 (2023).
2. Lozano, P. M., et al. “Anomalous Hall Effect at the Lifshitz Transition in $ZrTe_5$,” Phys. Rev. B 106, L081124 (2022).
3. Zhang, Y., Xu, C., Song, Y., et al. “Electronic Evidence of Temperature-Induced Lifshitz Transition and Topological Nature in $ZrTe_5$” Nat. Commun. 8, 15512 (2017).

*This research was supported by the Science Fund of the Republic of Serbia, 10925, Dynamics of CDW transition in strained quasi-1D systems - DYNAMIQS

Synthesis and Quantum Chemistry Evaluation of Hydrazones Bearing 5-Oxo-1-(4-(phenylamino)phenyl)pyrrolidine Moiety

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Abstract. The pyrrolidin-2-one scaffold has been associated with a vast range of biological activities and is one of the essential nitrogen-containing pharmacophores present in approved commercial drugs. Pyrrolidine moiety provides benefits in drug design because of the ring's unconstrained conformation, which may be locked and tuned with the suitable substituents [1]. Hydrazone derivatives, which biological activity is associated with the presence of the active azomethine pharmacophore, constitute another significant class of biologically active compounds in medicinal and pharmaceutical chemistry. Sixteen target hydrazone derivatives were synthesized from 5-oxo-1-(4-(phenylamino)phenyl)pyrrolidine-3-carbohydrazide and various aldehydes bearing aromatic and heterocyclic moieties and acetophenones [2]. Quantum chemistry simulations were carried out to evaluate their probable activity. Optimization of ground state molecular structure for several conformers was carried out by means of *Gaussian16* [3] software using density functional CAM-B3LYP method and 6-31G(d,p) basis set supplemented with polarization functions (d,p). Solvation effects (water surrounding) were estimated using PCM method. Electronic excitations were simulated using semiempirical TD method (for singlets). For population of excited lowest electronic state using transition $S_0 \rightarrow S_1$, in all cases dominant and most significant electron jump is not of homo→lumo type, but homo-1→lumo or homo→lumo+1. For hydrazones, two important factors must be pointed out. Firstly, phenyl ring of hydrazone related to the core through the bridge [–NH–] is present in out-of-plane (not-fixed) orientation and could occupy several positions. Re-switching between such two positions by passing an energetical barrier could be treated as the realization of key for switch on/off between several electronic clouds. Secondly, for several compound models, specific orientation of carbonyl group and neighbour [–N=N–] bridge allows to create pseudo-conjugated ring [..O=C–N-N–C–H..] which could be implemented into core π-conjugated system. Substituents related to the core allow to express well-defined charge-transfer (CT) transition or partial charge redistribution between fragments. Specific orientation of carbonyl group and neighbour [–N=N–] bridge allows to create pseudo-conjugated ring [..O=C–N-N–C–H..]. Substituents related to the core allow to express well-defined charge-transfer (CT) transition or partial charge redistribution between fragments.

REFERENCES

1. Albratty, M., *J. Saudi Chem. Soc.* **26**, 101509 (2022).
2. Zubrickė, I., Jonuškienė, I., Kantminienė, K., Tumosienė, I., and Petrikaitė, V., *Int. J. Mol. Sci.* **24**, 16804 (2023).
3. Gaussian 16, Revision C.01, M. J. Frisch, et al. Gaussian, Inc., Wallingford CT, 2019.

Electronic and Vibrational Properties of Iron-Doped Talc - Magnetic 2D Natural Material

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Abstract. Magnetic 2D materials have been a topic of great interest due to the potential for applications in spintronics. One of the biggest barriers to their implementation into future technologies has been their lack of ambient stability. This issue can be overcome through the use of natural 2D materials. [1]. Talc is a phyllosilicate found abundantly in nature with the chemical formula Mg3Si4O10(OH)2. It can be made into monolayers through processes such as mechanical and liquid phase exfoliation. A single layer of talc consists of [MgO4(OH)2] octahedra in between parallel sheets of [Si2O5] tetrahedra. Some iron-rich phyllosilicates, such as minnesotaite, have been found to occur naturally, which points towards the stability of such systems. While talc is naturally non-magnetic, the Mg cations can be substituted with Fe cations through broad beam irradiation [2]. In this research, we use computational methods based on density functional theory, as implemented in the Quantum Espresso software package, to analyze the stability, structural changes, electronic and vibrational properties of iron-doped talc. [3] Both of the inequivalent octahedral substitution sites for Mg were considered. Cell optimizations were performed to find the most energetically favourable structures. Band structures and magnetic moments were calculated afterwards. Band structure analysis showed a smaller band gap in the iron-doped talc compared to the undoped bulk, putting iron-doped talc in the semiconductor range. Finally, vibrational analysis was conducted for comparison with experimental Raman measurements. Iron-doped talc has the potential to become a new material for use in various applications through its demonstrated stability and ferromagnetic properties.

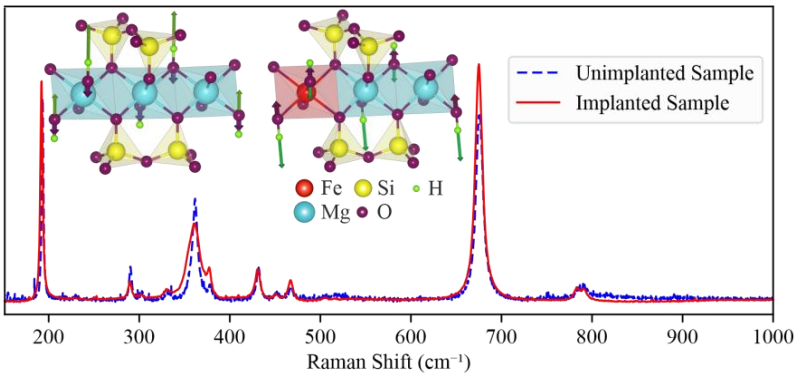

FIGURE 1. Raman spectrum of implanted and pure talc. Displace pattern for characteristic OH mode

REFERENCES

1. Khan M.Z. et al. *Adv. Phys. Res.*, **2**: 2300070. (2023).
2. Ion implantation in phyllosilicates, Khan M.Z. et al. *in preparation* (2025).
3. Giannozzi P. et al *J. Phys.: Condens. Matter* **21** 395502. (2009).

Towards numerically exact computation of conductivity in the thermodynamic limit of interacting lattice models

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Abstract. Recent works show that the ground state phase diagram of the square-lattice Hubbard model features a quantum critical line that passes through zero coupling at zero doping. At this point Boltzmann theory and the Kubo bubble [1] predict a linear-in-temperature resistivity down to the lowest accessible temperature yet there is a strong quantitative disagreement between the two, bringing into question the correctness of these theories. In this poster we present the results of our recent work [2] in which we develop and apply two different state-of-the-art methods for the calculation of dynamical response functions in interacting lattice models. We compute the dc conductivity in the weakly coupled Hubbard model in the thermodynamic limit in a fully controlled way without the analytical continuation. By comparing our methods to the Boltzmann theory we show that the latter leads to the quantitatively incorrect results due to the application of additional approximations. We show that vertex corrections have a significant impact on the dc conductivity results even at weak coupling and remain at a constant ratio to the Kubo bubble (as the coupling goes to zero).

REFERENCES

1. Vučičević, J., Predin, S., and Ferrero, M., in *Physical Review B*, **107**, 155140 (2023).
2. Kovačević J., Ferrero M., and Vučičević J., *preprint*, arXiv:2501.19118 (2025)

Diversification of Primary Mesenchymal Stromal/Stem Cell Populations at the Single-Cell Level Using Raman Spectroscopy

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Abstract. As a promising optical technique for application in biomedicine, Raman spectroscopy has been used for stem cell analysis, whereby the largest number of studies was based on the examination of the differentiation status of mesenchymal stromal/stem cells (MSCs) [1,2]. Namely, MSCs represent a diverse population of multipotent precursors that reside in many tissues. They have been isolated from various tissues and organs including bone marrow, adipose tissue, teeth, amniotic fluid, umbilical cord, tendon, etc., and due to simple and non-invasive isolation procedures MSCs are considered a valuable alternative source for cell replacement therapies. The main features of these cells are the ability to self-renew and the differentiation into several types of mature cells such as osteoblasts, adipocytes, chondrocytes under in vitro conditions. However, there is no precise marker that can be used to isolate and characterize this cell population, which significantly hinders further progress in potential application of these cells for therapeutic purposes. Therefore, our goal was to investigate the use of Raman spectroscopy to characterize biochemical profile of MSCs at single-cell level. In this study primary human MSCs derived from bone marrow (BM-MSCs) of five healthy pediatric donors collected during allogenic transplantation were analyzed. By using standard biological tests related to the MSCs features such as adherence, phenotype, clonogenicity, proliferation rate, pluripotency and multilineage differentiation potential variations between these donors were not detected. Raman spectroscopy analysis of MSCs at the single-cell level revealed a similar biochemical background of the tested samples. However, following the extensive principal component analysis (PCA), a clustering of MSCs populations was detected, particularly when the samples were analyzed in pairs. Obtained results indicate that Raman spectroscopy technique could provide valuable information for MSCs diversification and contribute to MSCs characterization, consequently accelerating their application in cell therapy [3].

REFERENCES

1. Bautista-González, S., Carrillo, González, N.J., Campos-Ordoñez, T., Acosta, Elías, M.A., Pedroza-Montero, M.R., Beas-Zárate, C., Gudiño-Cabrera, G., "Raman spectroscopy to assess the

differentiation of bone marrow mesenchymal stem cells into a glial phenotype". Regen Ther. 7; 24:528-535 (2023).
2. Geng J., Zhang W., Chen, C., Zhang, H., Zhou, A., Huang, Y, "Tracking the Differentiation Status of Human Neural Stem Cells through Label-Free Raman Spectroscopy and Machine Learning-Based Analysis". Anal. Chem. 93:10453–10461 (2021).
3. Kukolj, T., Lazarević, J., Borojević, A., Ralević, U., Vujić, D., Jauković, A., Lazarević, N., Bugarski, D., "A Single-Cell Raman Spectroscopy Analysis of Bone Marrow Mesenchymal Stem/Stromal Cells to Identify Inter-Individual Diversity". Int J Mol Sci. 28;23(9):4915 (2022).

Modeling Critical Temperature in Hg-based Cuprates Superconducting Material Using Multi-Property Descriptors

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Abstract. Superconducting materials, particularly mercury-based cuprates, exhibit high critical temperatures (T_c) and hold great potential for energy-efficient applications. However, accurately predicting T_c remains a challenge due to the complex interplay of structural and electronic properties. In this study, we employ a combination of machine learning (ML) techniques, including classification and regression models, to predict T_c and gain insights into key material properties. We apply the synthetic minority over-sampling technique to handle class imbalance in classification tasks, improving model generalization. For regression, we also utilize the sure independence screening and sparsifying operator with other ML model approach to derive low-dimensional descriptors that capture essential features governing superconductivity. By integrating these ML-driven techniques, we provide a systematic framework for analyzing superconducting materials and advancing the discovery of high-T_c compounds.

Structural, Morphological and Optical Properties of Er^{3+}-Doped $BaTiO_3$ Ceramics

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Abstract. Er^{3+}-doped $BaTiO_3$ (BTO) with perovskite ABO_3 structure is studied in terms of Er^{3+} substitution for Ba (A-site) and Ti (B-site) with different doping concentrations. Er^{3+}-doped BTO powders with different site substitutions and concentrations were prepared by solid-state reaction method. The as-made powder samples were pressed into a pellet shape and subsequently sintered at 1380 °C. The incorporation of Er^{3+} and the resulting properties are also strongly affected by sintering conditions. The morphological and optical properties of the synthesized samples were investigated by scanning electron microscopy, atomic force microcopy and Raman and photoluminescence spectroscopy, respectively. The impact of incorporated Er^{3+} on crystalline lattice vibration of BTO was investigated by Furrier transform (FT)-IR spectroscopy. Reflectivity measurement was used in far-IR range and in the mid-IR range - ATR-FTIR Transmittance. Together, the spectra cover the full range of normal BTO crystal modes. Scanning electron microscopy/energy-dispersive X-ray spectrometry (SEM-EDS) enables analysis and morphological characterization of surfaces of sintered samples. According to Ref.[1], the normal modes of BTO are assigned in FIG. 1b). As can be seen, the incorporation of Er^{3+} ions into the crystal lattice of $BaTiO_3$ caused an increase in the disorder of the crystal lattice and the appearance of a series of secondary modes. With increasing wt.% Er^{3+} modes show a slight red shift.

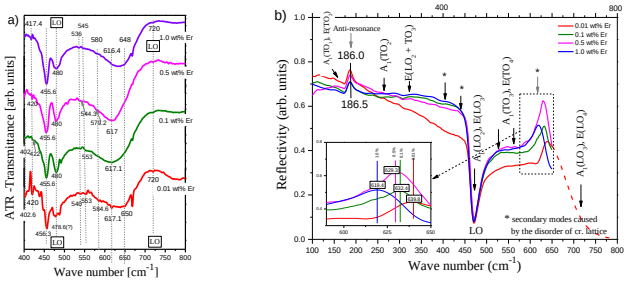

FIGURE 1. a) ATR-FTIR transmittance spectra of $BaTiO_3$:Er^{3+} (wt.% Er^{3+} = 0.01, 0.1, 0.5, 1.0) samples are presented with complementary reflectivity spectra, b) Together, the spectra cover the full range of normal crystal modes, from 100 cm^{-1} to 800 cm^{-1}, except soft mode $E(TO_1)$ that is at about 40 cm^{-1}.

REFERENCES

1. Meneses-Franco, A., Campos-Vallette, M., Octavio Vásquez, S. and Soto-Bustamante, E.A., *Materials* **11,** 1950 (2018).

$SrGd_2O_4$: Yb, Tm as Electrode Material for High Energy Density Electrochemical Supercapacitors

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Abstract. The current work aimed to examine the charge storage characteristics of $SrGd_2O_4$ and doped rare earth ions, specifically Yb^{3+} and Tm^{3+}. XRD, XPS, and FE-SEM with EDS were used to characterize these materials, which were made *via* straightforward sol-gel synthesis. The presence of Tm^{3+} and Yb^{3+} in the $SrGd_2O_4$ matrix with a consistent element distribution was verified by characterization. Pure $SrGd_2O_4$ and SrGd2O4:Yb4Tm1 charge storage behavior in different electrolytes was investigated in detail. Both electrode materials demonstrated large electrochemical potential windows in aqueous 6M KOH (1.7 V), necessary for supercapacitors to reach high specific energy. Additionally, compared to an undoped $SrGd_2O_4$ sample, $SrGd_2O_4$:Yb4Tm1 showed a significantly stronger charge storage effect in 6M KOH electrolyte, with nearly twice as high specific capacitance values. Matrix $SrGd_2O_4$ had the most effect on the electrochemical window, but rare earth dopants (Yb^{3+} and Tm^{3+}) had the greatest effect on specific capacitance. In electrochemical impedance spectroscopy tests, a significant decrease in total resistance demonstrated improved charge storage properties of $SrGd_2O_4$:Yb4Tm1. The $SrGd_2O_4$:Yb4Tm1 electrode in 6M KOH demonstrated a specific capacitance of 143 F g^{-1} and a specific energy of 12.5 Wh kg^{-1} at 0.6 A g^{-1} about the two-electrode GCD experiments. These results showhow rare earth ion doping can improve $SrGd_2O_4$'s energy storage capabilities, opening up exciting possibilities for the creation of high-performance supercapacitors.

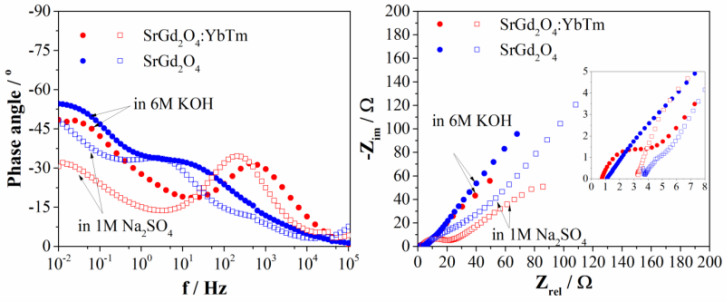

FIGURE 1. Electrochemical impedance spectroscopy measured at -1 V; Bode (left) and Nyquist (right) plot of investigated materials in 6M KOH and 1M Na_2SO_4.

ESUO-Serbia Section of Optical Society: Ten Years of Activities

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Abstract. ESUO-Serbia is a section of Optical Society of Serbia established in 2016 after the invitation by Prof. Dr. Dr. h.c. Ullrich Pietsch, the president of European Synchrotron and Free Electron Laser User Organization (ESUO). Although the Serbian synchrotron user community is rather small, it includes 30 to 35 active researchers, the research topics are diverse ranging from atomic and molecular physics and material sciences to chemistry and biology. During 2019 the first regional meeting of ESUO had been organized in Belgrade as a satellite meeting of The International School and Conference on Photonics. From the beginning of its activities, ESUO-Serbia maintains the web site [1] that includes the latest news from the community, papers published and projects performed by domestic researchers. Also, it provides links to the relevant documents and events. Some of our excellent researchers have been recruited to be beam-line scientists in such known synchrotron facilities as Diamond, DESY, ALMA and SOLEIL In 2024 the NEPHUEWS project [2] has been successfully launched and Serbia has been chosen among eight countries to be in the front line of beneficiaries.

FIGURE 1. The ESUO-Serbia web page http://uranus.ipb.ac.rs/~esuo-serbia/index.html .

REFERENCES

1. http://uranus.ipb.ac.rs/~esuo-serbia/index.html
2. https://beamtime.eu/programmes-support/ .

Neutrons and Photons Elevating Worldwide Science (NEPHEWS) – Trans-National Access For Excellent Curiosity Driven Research

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Abstract. NEPHEWS – the Neutrons and Photons Elevating Worldwide Science – is an Horizon Europe Co-funded project-based access program targeting new and non-expert users and user communities, driven by the neutron and photon European user communities [1]. It delivers access to the world-class collective of Europe's premiere open advanced neutron, synchrotron and free-electron laser complementary research infrastructures (RI), to promote curiosity driven excellence in research. The bottom-up User-to-User-oriented approach aims to build an integrated European RI landscape involving LEAPS and LENS consortia and their European scientific user communities. New and non-expert users receive in-depth hands-on expert training in twinning research experiments with expert-users, complimented with support in virtual access, workshops, schools and proposal writing. All build expertise, foster collaborations, and widen user access across the European Research Area. NEPHEWS specifically engages user and scientific communities of selected priority countries – of which **Serbia** is one – via outreach visits, priority access, and supporting political dialogue of national user communities with national funding authorities. The simultaneous effort for neutrons, free electron lasers and synchrotrons across Europe reduces the access barrier for using these techniques, sustains the user communities and helps to provide knowledge transfer between the user communities, to industry and the wider society researchers of neutron and photon sources worldwide is provided. Specific reference and statistics of the participation by Serbian researchers in worldwide neutron and photon facilities will be highlighted [2] along with participation in NEPHEWS programmes in the connected talk given in **Workshop 5:** Research opportunities at large scale user facilities.

REFERENCES

1. NEPHEWS project webpage, https://beamtime.eu/
2. Stankovski, M and Khotbehsara, F. A. P, "What is the size of the global light- and neutron source research communities?", Lund Institute of Advanced Neutron and X-ray Science, May 2024, https://www.linxs.se/news/article-series-i/size-of-the-global-light-and-neutron-source-communities

Transport Regimes of Holstein Polaron

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Abstract.

The transport characteristics of semiconducting materials are predominantly determined by the electron-phonon interaction. Different transport regimes can occur depending on the strength of this interaction and the temperature. There are three distinct regimes that manifest in specific scenarios. In the case when the electron-phonon interaction is weak, the carriers are delocalized and sometimes scatter on the phonons, placing the system within the conventional band transport regime. In contrast, when the electron-phonon interaction is strong and temperatures are high, the carriers become completely localized, and they occasionally hop from site to site, which is a phonon-activated process. If the electron-phonon interaction is strong but the temperature is very low, the carriers delocalize and form a very narrow band. This is known as the polaron band transport regime.

Numerous methods have been developed to calculate the carrier mobility in real materials. These methods typically rely on the assumption of either band transport or hopping transport. Consequently, these methods are occasionally used under conditions where the presence of any of the mentioned transport regimes is uncertain. Therefore, it is crucial to identify the range of validity of different transport regimes within the parameter space. Furthermore, it is important to determine if there are areas in the parameter space where carrier transport cannot be described by any of the three mentioned regimes.

This research tackles these questions by examining a prototype model with electron-phonon interaction, the Holstein model. In this work, we performed numerically exact calculations of the imaginary-time current-current correlation function of the Holstein Hamiltonian for a broad range of model parameters. These calculations were performed using a path-integral based Quantum Monte Carlo method [1]. We compared these results with the results obtained under the assumption of conventional band transport, small polaron hopping and polaron band transport. From this comparison, we identify the regions in parameter space where each of these transport regimes is valid. In some instances where examining current-current correlation functions in imaginary time is inconclusive, we enhance our analysis by utilizing real-time comparisons or by referencing published data on numerically exact dc mobilities [1, 2]. In summary, we observe that the parameter space is nearly entirely covered by the three specified transport regimes [3].

This research was supported by the Science Fund of the Republic of Serbia, Grant No. 5468, Polaron Mobility in Model Systems and Real Materials - PolMoReMa.

REFERENCES

1. Miladić, S., Vukmirović, N., *Phys. Rev. B* **107**, 184315 (2023).
2. Janković, V., *J. Chem. Phys.* **159**, 094113 (2023).
3. Miladić, S., Vukmirović, N., "Transport Regimes of Holstein Polaron", in preparation.

Saturation Isothermal Remanent Magnetization of Grapevine Leaves as a Proxy for Environmental Pollution

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Abstract. Magnetic particulate matter (PM) monitoring can be realized by magnetic parameters' determination. The magnetic parameters' measurements can represent the alternative method for identification of PM and potentially toxic elements (PTE) pollution in the environmental studies. Determination of magnetic parameters such as saturation isothermal remanent magnetization (SIRM) has been described as cost-effective, sensitive and non-destructive method for PTE pollution assessment which allows fast screening of magnetic PM pollution over large areas [1, 2]. Content of SIRM on leaf surface (an indicator of current pollution) was assessed in agricultural areas (conventional and organic vineyards). Main aim of our study [3] was to explore whether SIRM can be a proxy for magnetic PM pollution and associated potentially toxic elements (PTEs) in agricultural areas. Saturation isothermal remanent magnetization may represent a reliable proxy for assessing the ambient PTE pollution in the agricultural environment, and there were some differences between the distributions of SIRM throughout the grapevine season [3]. The leaf SIRM could pinpoint site-specific pollution in the vineyard ambient, suggesting that grapevine leaves can be used as biomonitors of PTE ambient pollution and leaf SIRM as a reliable representation for magnetic PM and some PTEs. The advanced principal component analysis showed that leaf SIRM was associated with PTEs of those sampling sites where higher concentrations were observed (near a metal foundry in a conventional vineyard and parcels not surrounded by the natural barriers and near the river in an organic one). Measurements of SIRM parameter can be recommended as user-friendly, fast and eco-sustainable techniques for determining magnetic PM and PTE pollution hotspots in agricultural ambient as pre-screening before more detail PTE pollution research.

REFERENCES

1. Salo, H., *Magnetic air quality monitoring using cryptogams*. In: M. Aničić Urošević, G. Vuković, M. Tomašević (Eds.), *Biomonitoring of air pollution using mosses and lichens, a passive and active approach, state of the art research and perspectives*, Nova Science Publishers, 2017, 195–228.
2. Winkler, A., Contardo, T., Vannini, A., Sorbo, S., Basile, A., & Loppi, S., *Magnetic Emissions from brake wear are the major source of airborne particulate matter bioaccumulated by lichens exposed in Milan (Italy)*. Applied Sciences, 2020, **10**, 2073.
3. Milićević, T., Relić, D., Aničić Urošević, M., Castanheiro, A., Roganović, J., Samson, R., Popović, A. Non-destructive techniques for the determination of magnetic particle and element contents in

grapevine leaves and soil as an eco-sustainable tool for environmentalpollution assessment in the agricultural areas. Environmental Monitoring Assessment, 2023, **195**, 858.

Antibacterial activity of visible light-driven photocatalytic nanocomposite suspension

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Abstract. In order to protect wall surfaces inside rooms, a photocatalytically active suspension was synthesized based on anionic clays [1, 2] doped with an optimal concentration of $(NH_4)_2WO_4$. After being thoroughly characterized, it was applied to facade paint (without the presence of titanium- dioxide) and photocatalytic activity was demonstrated. The suspension is intended for self-cleaning of indoor wall surfaces from various model pollutants and bacteria. The photocatalytic activity was proven using the model pollutant Methyl orange, which was later replaced by bacteria.
The bacterial culture *Acinetobacter baumannii*, a bacterial species resistant to many antibiotics, was used. This bacterium was selected for testing photocatalytic degradation because it possesses a threat to patients in hospitals with weakened immune systems, with the potential to cause serious illness and even death. The antimicrobial effect of the newly designed photocatalytic suspension was tested on two types of materials—on wall material and on facade paint used on indoor walls, which had previously been tested for photocatalytic activity using a model pollutant. Samples were carefully prepared in a sense that the photocatalytic suspension was first applied and dried and then the bacterial suspension was applied over it. The prepared samples were exposed to white LED radiation, and the number of bacterial colonies was determined after 24 and 48 hours from the start of irradiation. This experiment demonstrated the antimicrobial effect of the photocatalytic suspension on the clinical isolate *Acinetobacter baumannii* at the samples with applied facade paint.

REFERENCES

1. Miljević, B., van der Bergh, J.M., Vučetić, S., Lazar, D., Ranogajec, J., *Ceram. Int.* **43**, 8214–8221 (2017).
2. Cerc Korošec, R., Miljević, B., Umek, P., van der Bergh, J. M., Vučetić, S., Ranogajec, J., *Ceram. Int.* **46**, 6756-6766 (2020).

Luminomagnetic Fe_3O_4 Nanostructures for Biomedical Application: Synthesis, Characterization, and Antibacterial Properties

Dušan Milojkov[a], Ana Mraković[b], Vukosava Živković-Radovanović[c], Gvozden Jovanović[a], Nikola Vuković[a], Ivana Mikavica[a], Ksenija Radotić[d]

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Abstract. Luminomagnetic Fe_3O_4 nanostructures, which combine magnetic and optical properties, represent a promising material for a wide range of biomedical applications, including targeted drug delivery, magnetic resonance imaging, and hyperthermia [1]. In this study, we report the synthesis and systematic investigation of luminomagnetic Fe_3O_4 nanostructures with a rod-like morphology. The Fe_3O_4 nanostructures were synthesized using a reduction-precipitation method to achieve structures with controlled sizes and morphologies. Characterization of these nanostructures included field emission scanning electron microscopy (FESEM), X-ray diffraction (XRD), Fourier-transform infrared (FTIR) spectroscopy, as well as superconducting quantum interference device (SQUID) and fluorescence spectroscopy (PL) to analyze their magnetic and optical properties. The obtained nanostructures exhibit good magnetization along with light emission, making them suitable for *in vivo* biosensing and magnetic therapies. Additionally, antibacterial properties were tested on *S. aureus* cells, demonstrating that these nanostructures can also serve as antibacterial agents. This work highlights the potential of Fe_3O_4 nanostructures as multifunctional materials in bioengineering and biomedical devices, with applications in drug targeting, magnetic resonance imaging, hyperthermia treatments, and as innovative antibacterial agents.

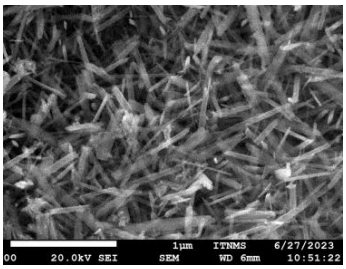

FIGURE 1. The structure and morphology of Fe_3O_4 nanorods.

REFERENCES

1. Castellanos-Rubio, I., et al. *ACS Appl. Mater. Interfaces* 14, 44, 50033–50044 (2022).

Modified Z-scheme Heterojunction of Polypyrrole/TiO_2: A Recyclable Photocatalyst for Azo Dyes Removal

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Abstract. It is well known that titanium dioxide is widely applied in photocatalysis regarding chemical and thermal stability, availability on the market, durability, and non-toxicity. Anatase, rutile, and brookite are three different crystalline modifications of TiO_2, whereby anatase is the most efficient for photocatalytic application. However, TiO_2 has some drawbacks: low adsorption power towards organic pollutants, high recombination rate during photocatalysis, and it can be excited only by UV light. Coupling TiO_2 with a conductive polymer, i.e. creating a conductive polymer/TiO_2 heterojunction, is a promising way to overcome these obstacles. Polypyrrole (PPy) is easy to prepare, stable, and possesses unique structure with delocalized π-electrons which contributes to the high mobility of charge carriers. In this work, PPy/TiO_2 composites with different amounts of PPy (0, 0.5, 1, 1.5, 3, and 5 wt.%) were obtained by physical mixing of hydrothermally synthesized TiO_2 and PPy prepared by the chemical oxidative polymerization. Prepared composites were characterized in detail by XRPD, FTIR, FESEM, EDS, UV/Vis, and BET methods. Photocatalytic activity of the samples was examined towards toxic textile azo dye Reactive Orange 16 (RO16) under simulated solar light, while photocatalytic efficiency was estimated by UV/Vis and TOC methods. XRPD results showed that TiO_2 was obtained with preserved nanoanatase structure in all the samples with crystallites of 26 nm. FTIR and EDS methods additionally confirmed presence of both, TiO_2 and PPy in all the nanocomposites. UV/Vis results revealed that band gap energy decreased with an increase in PPy content from 3.11(3) eV for single TiO_2 and 2.94(3) eV for 5%PPy/TiO_2. Prepared nanocomposites demonstrated excellent photocatalytic activity, while 1%PPy/TiO_2 was the most efficient by completely degrading RO16 dye after 120 min under simulated solar light. Such high efficiency was reached since all relevant factors were well balanced: sufficiently small TiO_2 crystallites, well distribution of PPy particles in a composite, narrowed band gap (3.08 eV), and significant improvement in specific surface area (61.71 $m^2\ g^{-1}$) compared to the single TiO_2 (36.46 $m^2\ g^{-1}$). Therefore, it can be concluded that the optimal content of PPy in the nanocomposite is 1 wt.%. Moreover, by performing several cycles of photocatalysis the reusability of the 1%PPy/TiO_2 was confirmed since no decrease in efficiency was observed. Finally, the photocatalytic degradation mechanism of RO16 in the presence of 1%PPy/TiO_2 was examined based on scavenger tests and thermodynamic calculations. Two important facts were found: (i) the mechanism can be well described by a slightly modified Z-scheme heterojunction, and (ii) PPy plays an active role in the process of photocatalysis by opening a new reaction pathway.

Topological origin of superconductivity in twisted bilayer WSe_2

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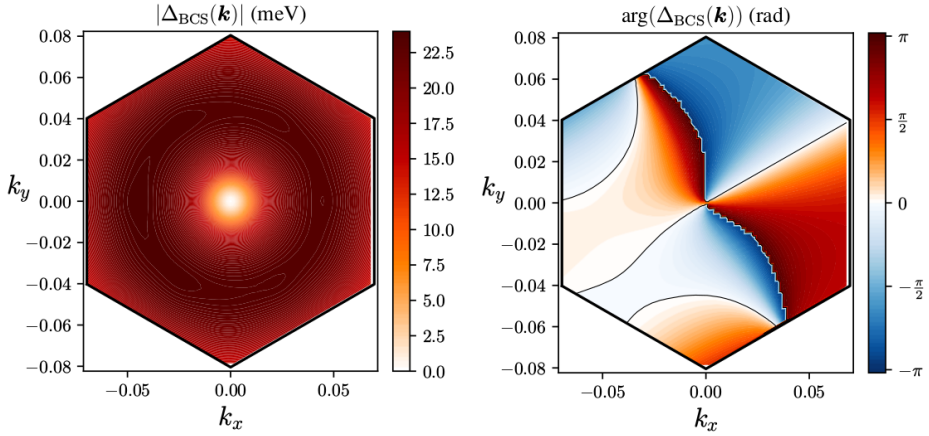
Abstract. The experimental discovery of superconductivity in twisted bilayer WSe_2 [1, 2] was followed by intense theoretical efforts to explain the effect. In particular, the physics at the angle equal to 3.65^o was addressed by traditional approaches based on the Kohn-Luttinger mechanism, but the explanation of the superconductivity and the phase diagram, at this twist angle, is unsatisfactory. By drawing the analogy with the topological pairing in the context of fractional quantum Hall physics, we discuss the possibility that the superconductivity around the half-filling of each of two Chern bands for two valley degrees of freedom is caused by special correlations in the topological bands and effective dipolar (higher-monopole) physics. The topological correlations in the BCS mean-field approach are incorporated via a special constraint that reflects their incompressible nature. The resulting superconductivity is topological and relevant only for the special fillings of the bands in accordance with the experiment. We also discuss the underlying physics of a correlated insulator for the two half-filled bands that was detected at higher values of the potential difference between the two layers of WSe_2 at the same twist angle.



REFERENCES

1. Xia, Y., Han, Z., Watanabe, K. et al. *Superconductivity in twisted bilayer WSe_2*, Nature **637**, 833–838 (2025).
2. Guo, Y., Pack, J., Swann, J. et al. *Superconductivity in 5.0° twisted bilayer WSe_2*, Nature **637**, 839–845 (2025).

Topological pairing of composite fermions in FQHE systems

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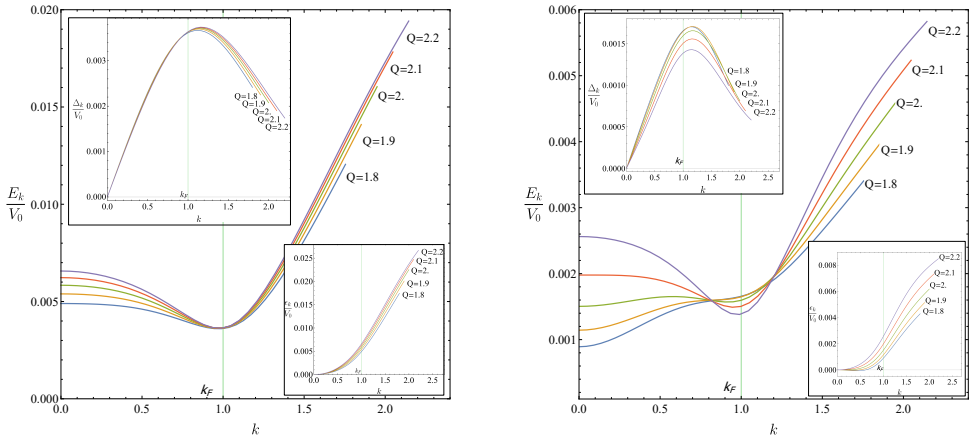
Abstract. The discovery of the fractional quantum Hall effect (FQHE) of electrons at filling factor 5/2 introduced the concept of a paired state of underlying composite fermion quasiparticles. This so-called Pfaffian state supports non-Abelian statistics and it is important to understand the exact mechanism that leads to such a state. We analyze ways to create Pfaffian by using the dipole representation of FQHE systems: the bosonic at filling factor one and half-filled Landau levels of electrons. We identify Hamiltonian(s), based on the constraints that characterize the representation in an enlarged space, that lead to Pfaffian phase in a mean-field approach, and discuss the role and nature of a critical point, in the phase space, that accompanies the Pfaffian physics [1].



(**a**) (**b**)

FIGURE 1. Bogoliubov quasiparticle dispersions in the lowest (a) and the second (b) Landau level. In top-left insertions are plotted the order parameters, and in bottom-right are effective dispersions for corresponding Landau levels.

REFERENCES

1. Nešković, N., Vasić, I., Milovanović, M. V., *Topological pairing of composite fermions via criticality*, Phys. Rev. B **110**, 125107, (2024).

Computational Assessment of Polymer-Based Drug Delivery

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Abstract. Dermal forms are promising drug delivery systems due to their many advantages and suitable applications. The physico-chemical characteristics of polymers affect their applicability profile as part of dermal pharmaceutical forms. Hansen's three-dimensional solubility (HSP) concept can be used to preliminary assess the potential of tested polymers as drug carriers [1]. It is known that the dispersive (δ_d), polar (δ_p), and hydrogen (δ_h) HSP components can determine the potential of polymeric carriers in effective drug delivery. Using Hansen's three-dimensional concept, the characteristics of three selected synthesized polymers (PEG 400, PEG 600, PEG-modified with lauric acid) in the effective dermal delivery of the fluoxetine were evaluated. A sphere with (δ_d, δ_p, δ_h) coordinates is experimentally defined (δ_d = 16.5, δ_p = 12, δ_h = 7.7, *R*o = 6.3), representing the region with the desired polymer characteristics [2]. Only those compounds located within the defined HSP sphere (*RED* < 1) are considered to have an appropriate drug delivery profile. The HSP forces for selected polymers were determined in the HSPiP software.The obtained *RED* values indicated a better dermal drug delivery profile with PEG 400 and PEG 600 compared to their modification.

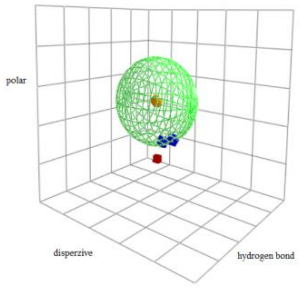

FIGURE 1. 3D solubility of the stratum corneum 32 °C and the position of the polymers obtained from HSPiP. The Center of the spheres shows the HSP values for the stratum corneum: δ_d = 16.5, δ_p = 12, δ_h = 7.7, *R*o = 6.3

REFERENCES

1. Cvetković, D., Dankulov, M.M., Bogojević, A., Lazović, S., and Obradović, D., *Chemometr. Intell. Lab. Syst.*, **251**, no. 105168 (2024).
2. Ezati, N., Roberts, S., Zhang, Q, and H. R. Moghimi, H.R., *Iran. J. Pharm. Res*., **19**, 572–578, (2020).

Murunskite: A Novel Platform for High-Tc Superconductivity Research with Intrinsic Magnetic Nanodomains

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Recently, we achieved a significant milestone by developing a reliable method for synthesizing high-quality single crystals of murunskite ($K_2FeCu_3S_4$) [1]. This entirely novel compound exhibits semiconducting behavior, as evidenced by resistivity and optical conductivity measurements–similar to superconducting cuprate parent compounds. Additionally, it shows antiferromagnetic-like ordering at 100 K. Structurally, however, murunskite is isostructural to metallic 122-type iron pnictides, making it a unique bridge between cuprates and ferropnictides – the only known families of high-temperature superconductors at ambient pressure.

In addition, murunskite undergoes a cascade of intriguing electronic and magnetic orderings: resulting in an antiferromagnetic transition around 100 K, followed by the onset of full magnetic and orbital ordering below 30 K [2]. The magnetism is exceptionally robust against structural disorder.

Given these unique properties, murunskite holds significant potential for future discoveries via tailored doping strategies. To explore this, we present several synthetic approaches involving substitution and doping with elements such as As, Se, Cr, Co, and Ni. The newly synthesized single crystals were thoroughly characterized using a range of experimental techniques, including magnetic susceptibility, resistivity measurements, and optical spectroscopy.

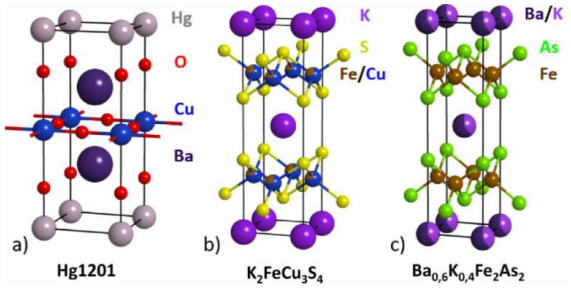

FIGURE 1. Crystal structure of a) cuprates, b) murunskite and c) pnictides

1. D. Tolj, T. Ivčić, I. Žiković, K. Semeniuk, E. Martino, A. Arkap, P. Reddy, B. Klebel-Knobloch, I. Lončarić, L. Forro, N. Barišić, H. M. Ronnow, D. K. Sunko, *Synthesis of murunskite single crystals: A bridge between cuprates and pnictides, Applied Materials Today, 24, 101096 (2021)*
2. I. V. Perkov, N. V. Zubkova, D. V. Lisitsyn, D. Y. Pushcharovsky, *Crystal Chemistry of Murunskite, Geochemistry, 424, 385-387, 2009*

Investigation of Cu_xS layers on polymers surface by SEM and RAMAN

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Abstract. In this work, copper sulfide (Cu_xS) thin films were deposited on the surface of polyamide (PA) and polypropylene (PP) films using the chemical bath deposition (CBD) method. The CBD process was carried out by varying the 1-3 deposition cycles. The influence of the deposition cycles was studied to determine the optimal condition for the deposition process. Scanning electron microscopy (SEM) was used to evaluate the changes in the surface morphology of PA and PP after 2 or 3 cycles of Cu_xS film deposition. The thin copper sulfide films on the surface of PP and PA were well dispersed, relatively uniform, and consisted of randomly orientated particles.

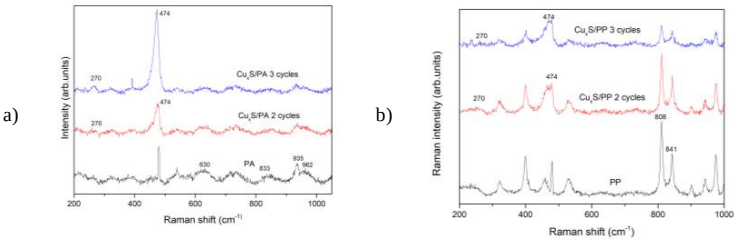

FIGURE 1. Raman spectra of the polymers: Cu_xS/PA (a) and Cu_xS/PP (b).

Raman spectrum of pure PA (Fig. 1a) shows C–C deformation mode at 630 cm^{-1}, band at 833 cm^{-1} is related to rocking CH_2, while the stretching mode of CH_2 is at 935 cm^{-1}, and 962 cm^{-1} corresponds to CO–NH vibrations. The Raman spectrum of PP (Fig. 1b) shows C–C stretching at 808 cm^{-1}, band at 841 cm^{-1} is related to the rocking CH_2, rocking at 972 cm^{-1}, and 998 cm^{-1} corresponds to CH_3 vibrations. Figures 1a and 1b show that the Raman spectra of copper sulfide film samples (deposited at 2 and 3 cycles) exhibit similar peak positions. The spectrum reveals a pronounced peak at 474 cm^{-1}, which is assigned to vibrational (stretching) modes from the covalent S–S bonds, and a much weaker peak at about 270 cm^{-1} attributed to the vibration of the Cu–S bond [1]. Raman analysis confirms the composition of the copper sulfide on the surface of PA and PP films.

REFERENCES

1. Ishii, M., Shibata, K., and Nozaki, H., *J. Solid State Chem.* **105,** 504–511(1993).

O_2 plasma modification of MoS_2 nanotubes for photocatalytic degradation of organic water pollutants

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Abstract. The dye contaminated wastewater is adversely affecting human health and the environment around the world. The issue can be resolved by photocatalytic degradation, which converts dyes into non-toxic compounds without producing secondary waste. In this work, we investigate the ability of MoS_2 nanotubes (NT) to decompose the rhodamine B (RhB) dye. MoS_2 NT synthesized by chemical vapor transport have high specific surface area, numerous S vacancies and favourable energy gap for visible light decomposition [1-2]. However, the initial degradation tests yielded poor results. The inert surface of MoS_2 NT was etched with O_2/Ar plasma which increased a number of catalytically active sites and introduced Mo-O bonds. UV-Vis and Raman spectroscopy, imaging techniques such as SEM, TEM and STM as well as the KPFM work function measurements verified the alteration. Simple MoO_3-MoS_2 system is formed, in which the reducibility of electron in the conductive band of MoS_2 increases, while the oxidability of hole in the valance band of MoO_3 also increases (Figure 1). We report over 90 % degradation efficiency, with the majority decomposing in the first 15 min of LED irradiation.

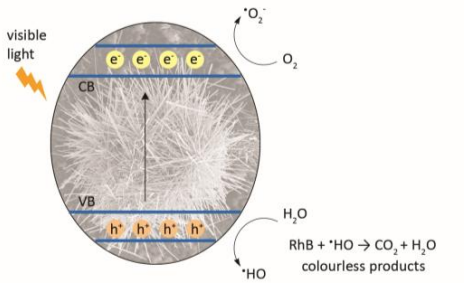

FIGURE 1. Shematic representation of photodegradation of RhB on MoS_2-MoO_3 NT.

REFERENCES

1. Remskar, M., Mrzel, A., Virsek, M. *et al.*, *Nanoscale Res Lett* **6**, 26 (2011).
2. Visic, B., Dominko, R., Gunde, M.K. *et al.*, *Nanoscale Res Lett* **6**, 593 (2011).

Effective Dielectric Function of a van der Waals Heterostructure Made of Two-Dimensional Materials Separated by Insulating Layers

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Abstract. Electron energy loss spectroscopy (EELS) is a commonly used experimental technique for investigating electronic and plasmonic properties of two-dimensional (2D) materials and van der Waals (vdW) heterostructures [1-3]. Following Ref. [4], we use the continued fraction (CF) method to derive a general expression for the effective 2D dielectric function of a vdW heterostructure made of 2D materials separated by insulating (isotropic or anisotropic) layers. The first objective is to obtain the EEL spectrum of such materials and (if possible) compare it with the available experimental data. We have extensive experience in the theoretical modeling of the experimental EELS data for free-standing (single and multilayer) graphene sheets obtained by scanning transmission electron microscope [5,6], as well as in the theoretical modeling of the experimental EELS data for monolayer graphene supported by different substrates [7-9]. As an implementation of the CF method, we evaluate the wake potential produced by a particle moving parallel to two graphene sheets separated by an isotropic insulator. For the first time, we assign the finite size of the gap between graphene and insulator in a graphene-insulator-graphene composite system. The second objective is to explore the effects of the graphene-insulator distance on the hybridization between the plasmon modes in graphene and phonon modes in the insulating substrate.

REFERENCES

1. Rossi, A. W., Bourgeois, M. R., Walton, C., and Masiello, D. J., *Nano Lett.* **24**, 7748 (2024).
2. Govyadinov, A. A., Konečná, A., Chuvilin, A., Vélez, S., Dolado, I., Nikitin, A. Y., Lopatin, S., Casanova, F., Hueso, L. E., Aizpurua, J., and Hillenbrand, R., *Nat. Commun.* **8**, 95 (2017).
3. Roslyak, O., Gumbs, G., and Huang, D., *Phys. E* **44**, 1874 (2012).
4. Lambin, Ph., Vigneron, J. P., and Lucas, A. A., *Phys. Rev. B* **32**, 8203 (1985).
5. Borka Jovanović, V., Radović, I., Borka, D., and Mišković, Z. L., *Phys. Rev. B* **84**, 155416 (2011).
6. Djordjević, T., Radović, I., Despoja, V., Lyon, K., Borka, D., and Mišković, Z. L., *Ultramicroscopy* **184**, 134 (2018).
7. Politano, A., Radović, I., Borka, D., Mišković, Z. L., and Chiarello, G., *Carbon* **96**, 91 (2016).
8. Politano, A., Radović, I., Borka, D., Mišković, Z. L., Yu, H. K., Farías, D., and Chiarello, G., *Carbon* **114**, 70 (2017).
9. Despoja, V., Radović, I., Politano, A., and Mišković, Z. L., *Nanomaterials* **10**, 703 (2020).

Spectroscopic and Morphological Properties of $Co_{0.9}Gd_{0.1}MoO_4$ Nanopowders

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Abstract. The glycine nitrate procedure (GNP) stands out as the most effective and reliable method for controlling the composition and morphology during the synthesis of $Co_{0.9}Gd_{0.1}MoO_4$ [1]. This combustion process ensures precise control over stoichiometry, homogeneity, and purity, allowing us to produce high-quality $Co_{0.9}Gd_{0.1}MoO_4$ with confidence. We conducted a thorough analysis of the samples synthesized using this method, employing a range of advanced characterization techniques, including Differential Thermal Analysis (DTA), X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FT-IR), Field Emission Scanning Electron Microscopy (FESEM), and nitrogen adsorption methods. The results revealed a high degree of anisotropy in the particles' shape and size, forming distinct agglomerates. Additionally, we observed significant differences in the microstructure, notably the development of well-defined plate-like crystals. Crucially, the color of the synthesized sample transformed from darker to lighter shades following thermal treatments. We also noted considerable changes in the dominant wavelength (in nanometers) and color purity between the initial sample and the sample heated to 1100 °C, primarily driven by variations in cobalt concentration. This highlights the effectiveness of the GNP in achieving controlled and reproducible synthesis outcomes.

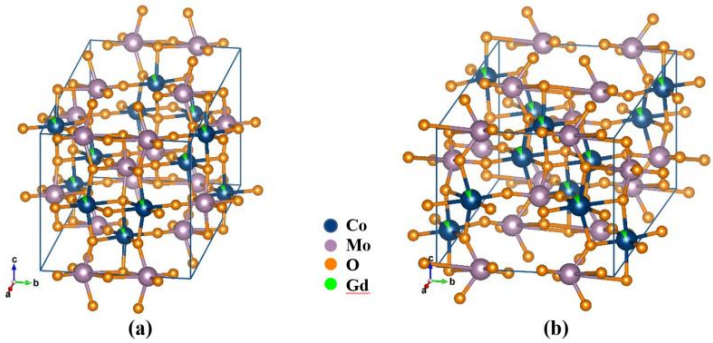

FIGURE 1. Structure of synthesized and calcinated samples at 450 and 1100 °C: a) α-$Co_{0.9}Gd_{0.1}MoO_4$ and b) β-$Co_{0.9}Gd_{0.1}MoO_4$.

REFERENCES

1. Rosić, M.; Zarubica, A.; Šaponjić, A.; Babić, B.; Zagorac, J.; Jordanov, D.; Matović, B. Structural and photocatalytic examination of $CoMoO_4$ nanopowders synthesized by GNP method, *Mater. Res. Bull.* **98**, 111–120 (2018), http://dx.doi.org/10.1016/j.materresbull.2017.10.015.

Ambient Dependence of Electrical Properties in Scalable Graphene-based Materials

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Abstract. We investigated ambient dependence of conductivity, carrier density and Hall mobility in different types of scalable graphene-based materials, each differing in thickness and prepared with different production methods. Two types of graphene dispersions were used to fabricate thin graphene films with the Langmuir-Blodgett method. Although both types of dispersions are produced with liquid-phase exfoliation (LPE), one is made by ultrasound-induced LPE (USLPE), and the other by electrochemical exfoliation (EE) [1]. The third production method is laser induction of graphene (LIG) [2]. Hall measurements were conducted on samples that were annealed prior to ambient exposure. We found that as the carrier density decreases, the mobility increases in all samples, similar to what was found before for CVD graphene [3], although the dependence follows a different exponent. The results also revealed a strong dependence of conductivity on film thickness. USLPE samples were affected the most by exposure to ambient conditions, which could be related to their small thickness and abundancy of edge sites. Although LIG demonstrated the lowest conductivity among the samples, it showed the highest stability under ambient conditions. This suggests that only the surface layers of LIG interact with surrounding molecules and ions, keeping the average carrier path unaffected.

This research was supported by the Ministry of Science, Technological Development and Innovation of the Republic of Sebia under contract number 451-03-136/2025-03/200026 and by the European Commission through project EMERGE (Emerging Printed Electronics Research Infrastructure H2020-INFRAIA-2020-1 (Grant agreement ID: 101008701)).

REFERENCES

1. S. Andrić, T. Tomašević-Ilić, L. Rakočević, D. Vasiljević-Radović, and M. Spasenović, Three Types of Films from Liquid-phase-exfoliated Graphene for Use as Humidity Sensors and Respiration Monitors, Sens. Mater. **34**, 3933 (2022).
2. J. Lin et al, Laser-induced porous graphene films from commercial polymers, Nature Comm. **5**, 5714 (2014).
3. F. Qing et al, A general and simple method for evaluating the electrical transport performance of graphene by the van der Pauw-Hall measurement, Sci. Bull. **63**, 1521 (2018).

Crystalline Structure Analysis via Channeling Rainbow Scattering

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Abstract. A new method for crystalline characterization based on the rainbow scattering effect is proposed. The most dominant effect in ion channeling is the existence of crystal rainbows [1], which can be easily used for morphological characterization. Our novel method simplifies the complex analysis of probing ions through a straightforward numerical calculation of rainbow lines, thereby greatly reducing analysis time. Depending on the crystal type [2], crystal rainbows exhibit unique shapes and sizes for each different crystal. Therefore, by conducting a simple morphological investigation of the calculated rainbow lines based on recorded angular distributions of channeled ions, we can confidently determine the crystal structure in question [3]. Additionally, impurities, defects, vacancies, and interstitials significantly influence certain parts of the rainbow pattern, which can be further used to identify these effects. This approach provides a fast, efficient, and reliable method for crystalline characterization, offering valuable insights into material properties and potential defects.

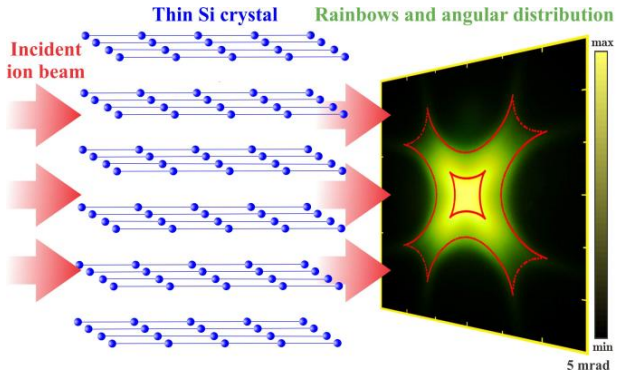

FIGURE 1. Ion channeling through thin oriented crystal and recorded angular distributions of channeled ions with corresponding angular rainbow lines.

REFERENCES

1. Nešković, N., Petrović, S., and Ćosić, M., *Rainbows in Channeling of Charged Perticles in Crystals and Nanotubes*, Cham: Springer, 2017, pp. 25-119.
2. Petrović, S., Nešković, N., Ćosić, M., Motapothula, M., and Breese, M. B. H., *Nucl. Instr. Meth. Phy. Res. B* **360**, 23-29 (2015).
3. Starčević, N., and Petrović, S., *Nucl. Instr. Meth. Phy. Res. B* **499**, 39-45 (2021).

Theoretical Prediction and Experimental Validation of Temperature-Dependent Raman Spectra of Doxorubicin

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Abstract Temperature-dependent Raman spectra of doxorubicin revealed a pronounced evolution of spectral features, with a notable crossover in peak intensities occurring between 100 K and 300 K. Theoretical Raman spectra of a single doxorubicin molecule were calculated using the ORCA program. The GOAT algorithm was used to identify isomers of neutral doxorubicin, doxorubicin hydrochloride, and its cationic form. The most stable structures were optimized, and harmonic vibrational frequencies and Raman activities were computed at the R2SCAN/def2-TZVP level of theory with D3 dispersion. Spectra for a doxorubicin dimer were also simulated. The observed temperature-dependent spectral features were successfully explained by resonant Raman calculations, which included spectral broadening, anharmonic scaling, and Duschinsky rotation effects. Theoretical predictions were compared with experimental data using the Python-based SARA program, showing excellent agreement across the studied temperature range.

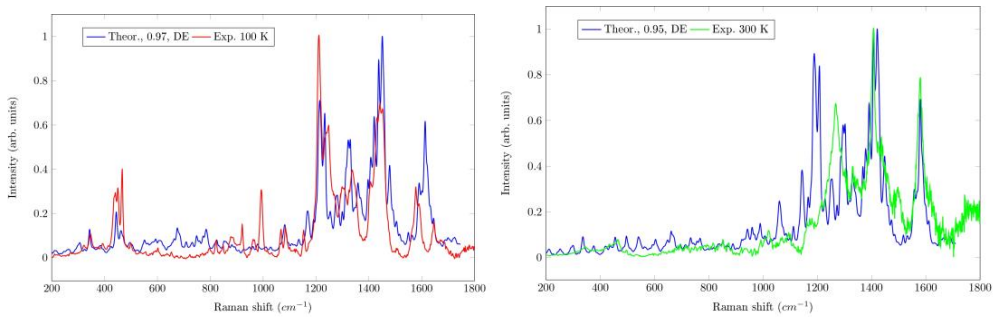

FIGURE 1. Experimental Raman and theoretical resonant Raman spectra of doxorubicin at 100K (left) and 300K (right).

Corrosion of Mn Coatings in a Salt Spray Chamber

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Abstract. Manganese coatings are excellent for cathodic corrosion protection of steel. From the literature review, it must be concluded that the most effective electrolytic additives used for electrodeposition of Mn are inorganic compounds, containing sulphur, selenium and tellurium. However, there is insufficient data on the Te compounds' influence on the electrodeposition of Mn coatings and their properties. Recently, the influence of some tellurium Te compound additives on the electrodeposition process of Mn coatings and their properties (structure, morphology, current efficiency, etc.) were studied [1–3]. In order to better identify the behaviour of electrolytic Mn coatings in protecting steel base against corrosion over a longer period of time, they have been tested in a salt spray atmosphere. Corrosion resistance of manganese coatings was evaluated gravimetrically according to the change in mass per area unit over time. The tests in a chamber of the salt spray showed that sample mass increased over time due to the formation of slightly soluble and insoluble corrosion products on the surface of the coatings. An accurate calculation of the corrosion rate according to the mass increase per area unit ($\Delta m/S$) requires the identification of corrosion products and their quantitative composition. The measurement results of coating mass increase are influenced by the dissolution of corrosion products themselves and their adhesion to the Mn coating. The corrosion products are formed quicker and in larger quantity on the surface of the Mn coatings deposited from the manganese-ammonium sulphate bath (MASB) in the range of cathodic current densities j_c = 5–10 A·dm^{-2}. These samples were removed from the salt spray chamber after ~ 144 h,when Mn coatings were fully corroded and corrosion damages to the steel substrate was visible. The corrosion of Mn coatings deposited at 15 A·dm^{-2} corrodedin 246 h. The mass of additionaly phosphated Mn coating initially decreased as the soluble phosphatic film was dissoloving first. The change in color over time resulting from the corrosion products formed on the surface of the Mn coatings was evaluated visually, after removing the testing samples from the salt spray chamber. For the longest period of time (even 546 h) corrosion products of Mn were not observed on the surface of phosphated Mn coatings. When the MASB temperature was increased, fewer corrosion products formed. The most corrosion-resistant Mn coatings were the ones deposited at 80 °C: their significant corrosion damage appeared only after 546 h.

REFERENCES

1. Sharma, R.K., Rastogi, A.C. and Singh, G., *Mater. Chem. Phys*. **84**, 46–51 (**2004)**.
2. Griskonis, E., Sulcius, A. and Zmuidzinaviciene, N., *J. Appl. Electrochem.* **44**, 1117–1125 (**2014)**.
3. Zmuidzinaviciene, N., Griskonis, E. and Sulcius, A., *Coatings*, **13**, 1617 **(2023)**.

Advances in Solid State Physics and New Materials (5; 2025; Beograd)

Book of abstracts / Advances in Solid State Physics and New Materials - 30 years of the Center for Solid State Physics and New Materials at the Institute of Physics Belgrade, 19 – 23 May 2025, Belgrade, Serbia; editors Bojana Višić and Andrijana Šolajić. – Belgrade: Center for Solid State Physics and New Materials, Institute of Physics, 2025 (Belgrade: SASA).

ISBN 978-86-82441-65-6

1. Advances in Solid State Physics and New Materials

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