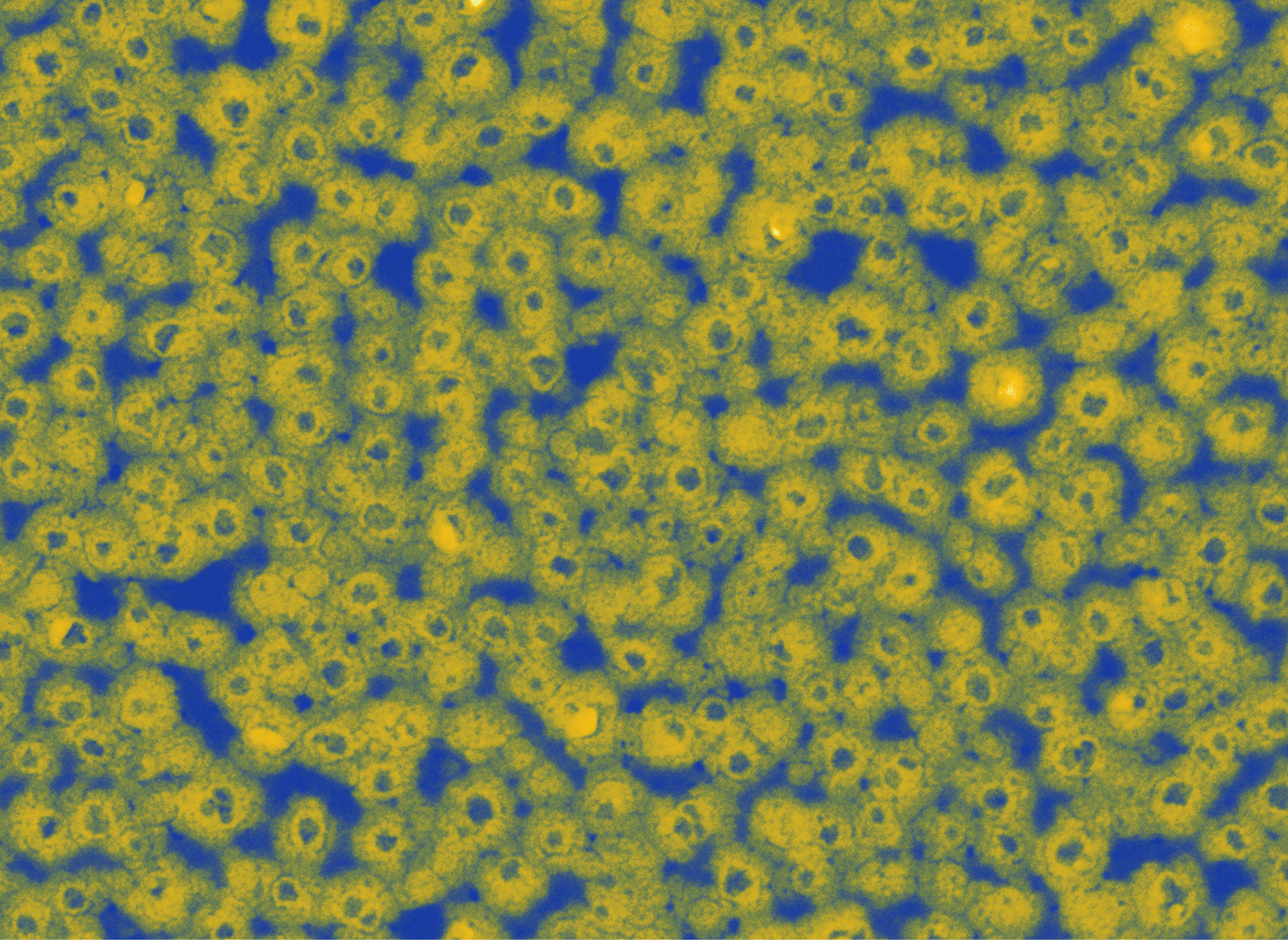

Nanoscience Institute
4th Workshop

CNRNANO
ISTITUTO NANOSCIENZE CONSIGLIO NAZIONALE DELLE RICERCHE

4th Meeting of the
Nanoscience Institute | Cnr Nano

June 05–06, 2025
Cnr Nano S3
Via Campi 213/a
Modena | Italy

Index

PRESENTATION

Welcome to the 4th Nanoscience Institute Workshop - *"Reconnecting, inspiring interactions"*

We are delighted to welcome you to the 4th Workshop of the Nanoscience Institute of the National Research Council (CNR), taking place on June 05–06, 2025, at CNR Nano in Modena. This event marks our first in-person gathering since 2018 and offers a long-awaited opportunity to reconnect as a scientific community, rekindle dialogue, and renew collaborations.

Following the successful editions in Matraia-LU (2010), Modena (2014), and Pisa (2018), this year's workshop celebrates our collective identity and promotes new interdisciplinary synergies across the institute. Over the course of two days, we will explore frontier topics in nanoscience — from quantum materials and advanced electron microscopy to THz photonics, nanoscale biosensing, and computational materials science. Special attention will also be devoted to the role of nanotechnology in addressing global challenges in energy, healthcare, and sustainability.

The scientific program includes oral presentations covering all major research areas within the institute, designed to promote knowledge exchange, stimulate discussion, and foster cross-disciplinary collaboration. Each session includes contributions from different research domains, deliberately structured to avoid compartmentalization and to encourage mutual awareness of the institute's full spectrum of activities. A large poster session will further enrich the discussions and promote informal interactions.

As part of the program's broader spirit of reconnection, the evening of the first day will feature a concert by the Apulian Youth Symphony Orchestra (AYSO), offered as a cultural interlude before the social dinner — a moment to celebrate our community in a different but equally meaningful register.

We gratefully acknowledge the support of our sponsors, whose contributions have made this event possible and who will also showcase their latest technologies and products during the workshop.

A special thanks goes to the CNR Nano staff for their dedication and invaluable effort in organizing this meeting.

Beyond its scientific content, this workshop serves as a meaningful occasion to reflect together on our strategic trajectory. It will offer a valuable opportunity to discuss how we envision the evolution of our institute and how we can reshape our organization to effectively respond to present and future challenges.

We look forward to stimulating discussions, renewed collaborations, and a shared commitment to advancing the frontiers of nanoscience.

Pisa, May 20th, 2025

Gaetano Scamarcio

Director of the Nanoscience Institute – CNR

PROGRAMME

Thursday June 05, 2025			
14.15 –14.45		**Opening Remarks and Institutional Greetings**	
14.45 - 16.00		**First Scientific Session | 12' presentation + 3' Q&A**	Parallel Session | Research support staff
	14.45 - 15.00	**O1.01 Giorgia Brancolini** - *Multiscale Computation for Biointerfaces: Advancing Biosensors & Nanomedicine in One Health*	
	15.00 - 15.15	**O1.02 Francesco Giazotto** - *Coherent caloritronics, energy management, and power generation in superconducting quantum circuits*	
	15.15 - 15.30	**O1.03 Daniele Varsano** - *Exploring Electronic Screening and Exciton Insulator Phases in 2D Materials*	
	15.30 - 15.45	**O1.04 Giovanni Bertoni** - *First demonstration of angular-momentum-resolved electron energy-loss spectroscopy*	
	15.45 - 16.00	**O1.05 Leonardo Viti** - *Fast THz frequency photodetectors and applications in quantum communication*	
16.00 - 16.30		**Coffee break**	
16.30 - 17.45		**Second Scientific Session | 12' presentation + 3' Q&A**	Parallel Session | Research support staff
	16.30 - 16.45	**O1.06 Marco Cecchini** - *Ultra-High-Frequency Surface Acoustic Waves for Advanced Microfluidics and Biosensing*	
	16.45 - 17.00	**O1.07 Eleonora Spurio** - *Photoexcitation of Cerium Oxide via Ultrafast X-ray Spectroscopy*	
	17.00 - 17.15	**O1.08 Michele Campisi** - *Advancing Quantum Computing with Quantum Thermodynamics (and vice-versa)*	
	17.15 - 17.30	**O1.09 Simone Zanotto** - *Optomechanical Metasurfaces*	
	17.30 - 17.45	**O1.10 Alberto Ghirri** - *Coherent coupling between magnons and microwave photons in planar magnet/superconductor hybrid systems*	
17.45 - 19.00		**First Poster Session**	
19.30 - 20.30		**Orchestra Concert by OrchestrAcademy AYSO @Arena Spazio Culturale (Viale A. Tassoni 8, 41121)**	
20.30		**Social Dinner @Arena Spazio Culturale**	

Friday June 06, 2025			
08.45		**Welcome**	
09.00 - 10.30		**Third Scientific Session | 12' presentation + 3' Q&A**	**Parallel Session | Research support staff**
	09.00 - 09.15	**O2.01 Stefano Pittalis** - *Density functional theory of magnetism*	
	09.15 - 09.30	**O2.02 Stefania Benedetti** - *Structure, electronic and plasmonic properties of amorphous transparent conducting oxide films for plasmonics in the mid-IR*	
	09.30 - 09.45	**O2.03 Ambra Del Grosso** - *Innovative Polymeric Nanosystems for Drug Delivery Across the Blood-Brain Barrier*	
	09.45 - 10.00	**O2.04 Sibilla Orsini** - *Light-based additive manufacturing for the management of complex fluids*	
	10.00 - 10.15	**O2.05 Claudio Puglia** - *Bridging the Gap: translating Quantum Research into commercial innovation*	
	10.15 - 10.30	**O2.06 Carlo Andrea Rozzi** - *Ultrafast Electron Dynamics in molecules, crystals, interfaces*	
10.30 - 11.00		**Coffee break**	
11.00 - 12.30		**Fourth Scientific Session | 12' presentation + 3' Q&A**	**Parallel Session | Research support staff**
	11.00 - 11.15	**O2.07 Sergio Pezzini** - *On-demand Hamiltonians in twisted graphene devices*	
	11.15 - 11.30	**O2.08 Alessandra Di Gaspare** - *Terahertz non-linear optics in van der Waals metamaterials: a bridge in the 24-60 um gap*	
	11.30 - 11.45	**O2.09 Andrea Secchi** - *Hole-spin qubits in germanium beyond the single-particle regime*	
	11.45 - 12.00	**O2.10 Federica Bianco** - *Electron particles to control electron waves in graphene systems*	
	12.00 - 12.15	**O2.11 Francesca Matino** - *Polymeric Piezoelectrics for Energy Harvesting Applications*	
	12.15 - 12.30	**O2.12 Luca Scaccini** - *Nano and microengineered chitosan-based scaffolds as a tuneable approach for peripheral nerve regeneration applications*	
12.30 - 13.30		**Lunch**	
13.30 - 14.45		**Second Poster Session**	
14.45 - 16.15		**Round table: Towards a Shared Strategy for the Development of the Nanoscience Institute**	
16.15 - 16.30		**Wrap-up and Closing remarks**	

Scientific Committee
Arrigo Calzolari
Stefan Heun
Paola Luches
Gaetano Scamarcio
Ilaria Tonazzini
Filippo Troiani

Organizing Committee
Maria Grazia Angelini
Maria Bartolacelli
Elisa Bolognesi
Davide Calanca
Susanna Cavicchioli
Giovanna Diprima
Luisa Neri
Massimo Rontani
Maddalena Scandola

Cover Image: STEM image of hollow copper oxide nanoparticles obtained by oxygen plasma treatment of self-assembled metallic nanoparticles. Courtesy of Paola Luches and Giovanni Bertoni (Cnr Nano S3).

Abstracts | Oral Presentations

[O1.01] Multiscale Computation for Biointerfaces: Advancing Biosensors & Nanomedicine in One Health

G. Brancolini[1], S. Corni[1,2], A. Mossa[1], A. Papalini[1], and G. Schifino[2]

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Multiscale computational modeling plays a crucial role in understanding and optimizing biofunctionalized surfaces for applications in biosensing and nanomedicine. In this talk, I will present an integrated computational-experimental framework to design and enhance biointerfaces, focusing on strategies for biomolecule anchoring, sensor stability, and functionalized nanomaterials [1].

I will discuss the optimization of biosensors for pathogen detection, including DNA aptamer-based strategies for viral diagnostics [2], as well as the development of biofunctionalized nanomaterials for antibacterial and therapeutic applications [3]. Attention will be given to the role of surface modifications in enhancing sensor sensitivity and the effectiveness of antimicrobial coatings. These advances align with the One Health approach, addressing interconnected human, animal, and environmental health challenges. By bridging computational modeling with experimental validation, this work contributes to the development of next-generation biosensors and bioengineered surfaces for healthcare and translational nanomedicine.

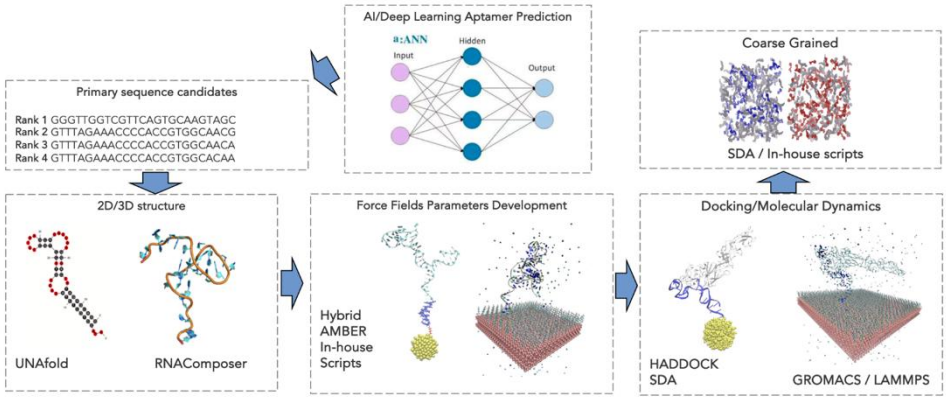

Fig. 1: The multi-scale protocol for optimizing aptamer-based biosensors to detect West Nile Virus

References

[1] S. Giberti, S. Dutta, S. Corni, M. Frasconi, and G. Brancolini. *Protein-Surface Interactions in Nano-Scale Biosensors for IL-6 Detection Using Functional Monolayers*. Nanoscale, 17, 4389 – 4399 (2025).

[2] A. Mossa and G. Brancolini. *Rational design of gold nanoparticles functionalized with aptamers for improved West Nile virus detection.* Under review (2025).

[3] A. Papalini, E. Passaglia, A. Sgarbossa, and G. Brancolini. *Computational Insights into Phosphorene-Protein Interactions for the Design of Antibacterial Nano-Composites.* To be submitted as invited article in *Molecules* (2025).

[O1.02] Coherent caloritronics, energy management, and power generation in superconducting quantum circuits

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The nascent discipline of *phase- coherent caloritronics* (derived from the Latin term "calor", meaning heat) is based on the ability to regulate thermal currents through the phase difference of the superconducting order parameter [1]. The goal is to conceive and develop thermal devices capable of managing energy transfer with precision comparable to charge transport in modern electronic components. This can be achieved by leveraging the macroscopic quantum coherence inherent in superconducting condensates, demonstrated through the Josephson and proximity effects. In this talk, I will first assess recent experimental results obtained in the development of heat interferometers and thermal rectifiers and examine several proposals for unconventional non-linear phase-coherent caloritronic devices, including thermal transistors, phase-coherent heat splitters, microwave refrigerators, thermal engines, and heat valves. Apart from being extremely compelling from a fundamental physics standpoint, these systems are expected to significantly influence numerous cryogenic microcircuits requiring energy management, potentially laying the groundwork for the emergence of electronic thermal logic.

Subsequently, I will evaluate the feasibility of generating power within superconducting quantum circuits. In this context, thermoelectric effects in metals are typically negligible due to the nearly perfect particle-hole (PH) symmetry near their Fermi surface. Additionally, thermo-phase effects and linear thermoelectricity in superconducting systems have only been recognized when PH symmetry is intentionally disrupted, as thermoelectric effects were thought to be unattainable in superconductors. I will demonstrate that Josephson tunnel junctions can exhibit significant *bipolar* thermoelectricity with a substantial thermal gradient due to spontaneous PH symmetry breaking [2]. When subjected to a considerable thermal bias, Josephson junctions display notable bipolar power generation, resulting from non-equilibrium-induced spontaneous PH symmetry breaking. Specifically, superconducting tunnel junctions may produce thermopower approximately 10^5 times greater than the linear Seebeck coefficient of a normal metal, making them exceptionally well-suited for application in superconducting quantum technology through the implementation of engines, power generators, electronic devices, memories, radiation sensors, and switches.

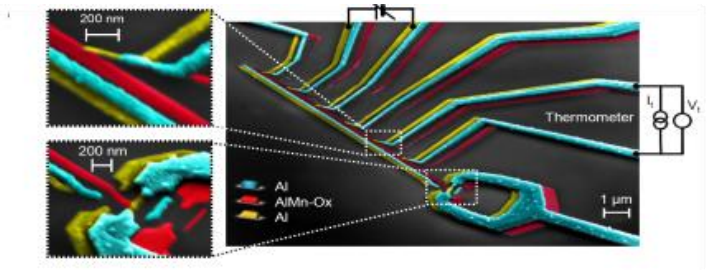

Fig. 1: Thermal superconducting quantum interference proximity transistor.

References

[1] A. Fornieri and F. Giazotto. *Towards phase-coherent caloritronics in superconducting circuits.* Nat. Nanotechnol. 12, 944 (2017).

[2] G. Germanese, F. Paolucci, G. Marchegiani, A. Braggio, and F. Giazotto. *Bipolar Thermoelectric Josephson Engine*, Nat. Nanotechnol. 17, 1084 (2022).

[O1.03] Exploring Electronic Screening and Exciton Insulator Phases in 2D Materials

D. Varsano[1], A. Ferretti[1], C. Cardoso[1], G. Sesti[1], M. D'Alessio[2,1], P. D'Amico[1], E. Molinari[2,1], and M. Rontani[1]

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Two-dimensional (2D) materials have attracted increasing attention in the last years due to their potential application in optoelectronic devices. Their reduced electronic screening, a consequence of dimensionality effects, makes them an ideal platform for investigating collective excitations such as excitons and plasmons, as well as quantum phenomena driven by electron correlation. This includes the possibility of spontaneous exciton generation and the realization of the excitonic insulator phase, a permanent Bose-Einstein condensate of excitons, which collectively sustain a many-body gap reminiscent of the exciton binding energy.

In this talk, I will present our group's effort in developing algorithms for accurately evaluating electronic screening in low dimensional systems using first principles approaches based on many-body perturbation theory [1,2,3,4] and I will survey theoretical predictions and interpretation of recent experimental findings that point to the emergence of exciton insulator phases in selected 2D materials [5,6]. Finally, I will outline future directions in the study of collective excitations in reduced dimensionality materials.

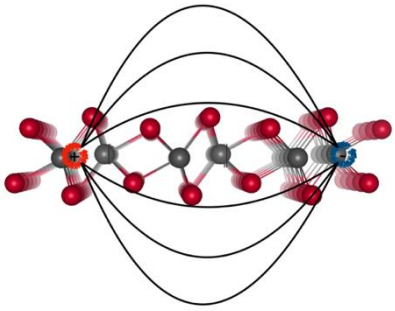

Fig. 1: Schematic representation of electron-hole interaction in WTe2 monolayer

References

[1] A. Guandalini, P D'Amico, A Ferretti, and D. Varsano. *Efficient GW calculations in two-dimensional materials through a stochastic integration of the screened potential.* npj Computational Materials 9, 44 (2023).

[2] G. Sesti, A. Guandalini, A. Ferretti, P. D'Amico, C. Cardoso, M. Rontani, and D. Varsano. *Accurate description of the long-range limit of the polarization in 2D metallic systems.* In preparation.

[3] A. Guandalini, D. A. Leon, P. D'Amico, C. Cardoso, A. Ferretti, M. Rontani, and D. Varsano. *Efficient calculations via interpolation of the screened interaction in momentum and frequency space: The case of graphene.* Phys. Rev. B 109, 075120 (2024).

[4] D. Sangalli, et al. *Many-body perturbation theory calculations using the yambo code.* Journal of physics: Condensed matter 31, 325902 (2019).

[5] B. Sun, et al. *Evidence for equilibrium exciton condensation in monolayer WTe_2.* Nature Physics 18, 94-99 (2022).

[6] D. Varsano, M. Palummo, E. Molinari, and M. Rontani. *A monolayer transition-metal dichalcogenide as a topological excitonic insulator.* Nature nanotechnology 15, 367-372 (2020).

[O1.04] First demonstration of angular-momentum-resolved electron energy-loss spectroscopy

G. Bertoni[1], E. Rotunno[1], P. Rosi[1], G. C. Gazzadi[1], S. Frabboni[2], and V. Grillo[1]

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Electron energy-loss spectroscopy (EELS) in transmission electron microscopy (TEM) is an essential tool for probing electronic transitions at atomic resolution. However, conventional EELS directly access the transferred linear momentum. We demonstrate here the first experimental realization of orbital angular momentum resolved EELS (or OAM-EELS), where an electron optical OAM sorter enables simultaneous energy and OAM dispersion, allowing direct measurement of rotational symmetries in atomic transitions. By applying this technique to the B K-edge of hexagonal boron nitride (h-BN), we achieve clear separation of the π and σ antibonding transitions, which are overlapped in conventional EELS.
Our experimental setup consists of a TEM (Thermo Fisher Scientific) with a post-column EELS spectrometer (Gatan, inc.) and a custom-built electrostatic OAM sorter [1] with two phase elements (S1 and S2) positioned after the specimen (Fig. 1a). These elements perform a log-polar conformal transformation, mapping OAM states onto the *y*-axis for detection. The system was operated with a 5.4 mrad convergence semi-angle (probe size ≃0.27 nm), which optimizes the tradeoff between spatial resolution and aberration minimization in the sorter. The OAM-EELS spectra were recorded at the B K-edge, where the 1s → π* and 1s → σ* transitions result in different OAM quantum numbers ($m = 0$ and $m = \pm 1$, respectively) (Fig. 1b). A zero-loss OAM-EELS spectrum in vacuum was acquired to establish the point spread function (psf) of the sorter.
A fundamental challenge in OAM-EELS is inelastic delocalization, where scattering broadens the measured OAM distribution, leading to an overlap of distinct electronic transitions. To mitigate this effect, we employed model-based spectral deconvolution. A simple Monte Carlo approach was used to simulate inelastic scattering events and their contributions to the OAM spectrum, and the experimental OAM-EELS spectra were then refined using multiple least-squares fitting. This deconvolution successfully separated the two components (Fig. 1c-e). A residual signal from π* transitions were observed at $m \neq 0$, reflecting the interplay between selection rules and delocalization effects. Despite the success of this approach, we propose several strategies for further improvement: i) The OAM sorter introduces aberrations at large scattering angles, limiting resolution. Improved fabrication techniques for the phase elements could reduce distortions permitting to work at larger angle to reduce probe size. ii) Introducing a limiting aperture at the sorter plane could selectively filter high angle scattering contributions, reducing the broadening in the measured OAM spectrum. iii) Neural networks could automate real-time OAM sorter alignment or OAM deconvolution, improving spectral fidelity and reducing operator dependence.
Our results establish OAM-EELS as a new tool for electron spectroscopy, enabling direct access to electronic states' rotational symmetry. This technique extends the capabilities of electron spectroscopy, offering applications in orbital mapping, electron magnetic circular dichroism (EMCD) and magnetism [2], plasmonics, quantum materials, etc. [3].

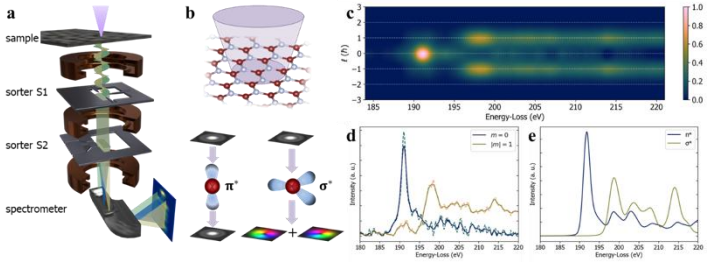

Fig. 1: a) Experimental setup to realize OAM-EELS double dispersion. b) Sketch of electron beam illumination on h-BN at 5.4 mrad and the electron wavefunction after single scattering on boron. c) Experimental OAM-EELS after model-based fitting to remove inelastic delocalization and psf of the sorter. d) experimental EEL spectra for $|m| = 1$ and (dashed lines are raw results, full lines are smoothed curves). e) Corresponding theoretical spectra.

References

[1] A. H. Tavabi, *et al. Experimental Demonstration of an Electrostatic Orbital Angular Momentum Sorter for Electron Beams.* Phys. Rev. Lett. 126, 094802 (2021).

[2] E. Rotunno, M. Zanfrognini, S. Frabboni, J. Rusz, R. E. Dunin Borkowski, E. Karimi, and V. Grillo. *Orbital angular momentum resolved electron magnetic chiral dichroism.* Phys. Rev. B 100, 224409 (2019).

[3] Submitted for publication. Research Square (preprint) (2024).

[O1.05] Fast THz frequency photodetectors and applications in quantum communication

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Sensitive photodetectors with large quantum efficiencies and broad dynamic ranges are essential for the implementation of photonic quantum platforms. In the Terahertz (THz) frequency range, with photon energies of few meV, the development of these devices is extremely challenging, owing to the lack of high-absorption materials and the concurring thermal effects that significantly impact their noise figure. In particular, enabling the statistical analysis of quantum intensity correlations in non-classical light sources, such as quantum cascade lasers (QCL) frequency combs, requires detectors with low noise equivalent powers (NEP). Recent advancements towards THz detectors with enhanced sensitivity include the use of devices based on two-dimensional (2D) materials, whose unique optoelectronic properties enable the activation of different physical mechanisms to detect far-infrared photons [1].

Here, we present various device architectures based on layered material heterostructures [2-4] to target a combination of large detection dynamic range, ultrafast response time, and low noise equivalent power, at frequencies around 3 THz, where state-of-the-art QCL frequency combs are available [5]. Perspectives of the application of our detection technologies in the field of free space optical [6]- and quantum-communications are provided and discussed.

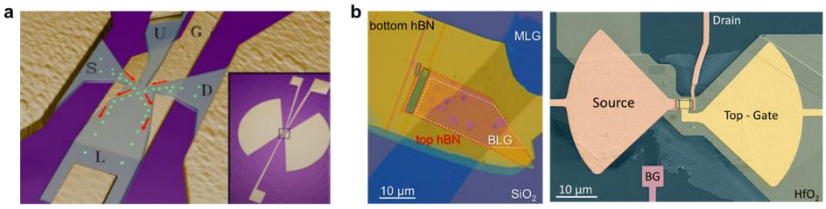

Fig. 1: High-performance terahertz photodetectors. (a) Schematic diagram of a graphene-based ballistic rectifier. (b) Optical and scanning electron micrograph (SEM) images of an antenna coupled tunnel field-effect transistor based on bilayer graphene.

References

[1] M.S. Vitiello and L. Viti. *Engineering THz-frequency light generation, detection, and manipulation through graphene.* Applied Physics Reviews 12 (1) (2025).

[2] L. Viti, L. Shi, K. Watanabe, T. Taniguchi, and M. S. Vitiello. *Quantum sensitive, record dynamic range Terahertz tunnel field-effect transistor detectors exploiting multilayer graphene/hBN/bi-layer graphene/hBN heterostructures.* Nano Letters (2025).

[3] L. Viti, O. Balci, J. Zhang, A. Meersha, A. C. Ferrari, and M. S. Vitiello. *Scalable Terahertz Room Temperature Photoreceivers Based on Large-Area Hexagonal Boron Nitride and Graphene Heterostructures.* Advanced Optical Materials, 2402100, (2025).

[4] L. Viti, V. Pushkarev, S. M. Abouzar Sarfraz, G. Scamarcio, and M. S. Vitiello. *Efficient large-area graphene p-n junction terahertz receivers on an integrated optical platform.* Small Methods (2025).

[5] M.S. Vitiello and P. De Natale. *Terahertz quantum cascade lasers as enabling quantum technology.* Advanced Quantum Technologies 5 (1), 2100082 (2022).

[6] A. Sorgi, M. Meucci, M. A. Umair, F. Cappelli, G. Toci, P. De Natale, L. Viti, A. C. Ferrari, M. S. Vitiello, L. Consolino, and J. Catani. *QCL-Based Cryogen-Free THz Optical Wireless Communication Link.* Laser & Photonics Reviews 2301082 (2025).

[O1.06] Ultra-High-Frequency Surface Acoustic Waves for Advanced Microfluidics and Biosensing

F. Lunardelli[1,2], M. Agostini[3], M. Gagliardi[1,2], S. Carpi[1,4], and M. Cecchini[1,2]

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Surface acoustic waves (SAWs) represent a highly promising technology for the development of lab-on-a-chip (LoC) devices, offering a versatile and scalable platform for biological fluid manipulation and biosensing. Their key advantages—low fabrication costs, scalable production, controllable physics, multifunctionality, and easy miniaturization—position SAWs as a strong candidate for replacing or complementing traditional laboratory facilities.

In particular, ultra-high-frequency SAWs (UHF-SAWs, 300 MHz–3 GHz) provide enhanced sensitivity to molecular adsorption and exceptional fluid manipulation capabilities, paving the way for next-generation LoC systems. By operating in this frequency range, UHF-SAWs enable highly reliable, fully automated, and high-performance biosensing applications.

This presentation will showcase our latest advancements in UHF-SAW-based microfluidics and biosensing, with a special focus on lab-on-chip applications. Key topics will include the detection of proteins, viruses, and bacteria, demonstrating the potential of UHF-SAW technology in biomedical diagnostics.

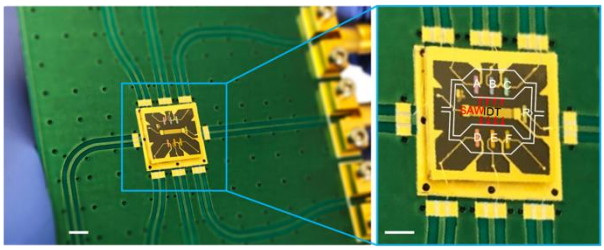

Fig. 1: A complete surface acoustic wave (SAW) biochip featuring six high-frequency resonator biosensors (A–F) and a low-frequency mixing interdigital transducer (SAW-IDT). In the zoomed image on the right, white lines outline the structure of the microfluidic chip layer.

References

[1] M. Gagliardi, M. Agostini, F. Lunardelli, L. Lamanna, A. Miranda, A. Bazzichi, A. Giuliana Luminare, F. Cervelli, F. Gambineri, M. Totaro, M. Lai, G. Maisetta, G. Batoni, M. Pistello, and M. Cecchini. *Surface Acoustic Wave-based Lab-On-a-Chip for the fast detection of Legionella pneumophila in water*. Sensors and Actuators B: Chemical (2023).

[2] M. Agostini, F. Lunardelli, M. Gagliardi, A. Miranda, L. Lamanna, A. Giuliana Luminare, F. Gambineri, M. Lai, M. Pistello, and M. Cecchini. *Surface-Acoustic-Wave (SAW) Induced Mixing Enhances the Detection of Viruses: Application to Measles Sensing in Whole Human Saliva with a SAW Lab-On-a-Chip*. Advanced Functional Materials (2022).

[O1.07] Photoexcitation of Cerium Oxide via Ultrafast X-ray Spectroscopy

E. Spurio[1], S. Pelatti[2,1], D. Catone[3], P. O'Keeffe[4], S. Turchini[3], G. Ammirati[3], F. Paleari[1], D. Varsano[1], S. Benedetti[1], A. di Bona[1], S. D'Addato[2,1], Y. Jiang[5], P. Zalden[5], Y. Uemura[5], H. Wang[5], D. Vinci[5], X. Huang[5], F. Lima[5], M. Biednov[5], D. Khakhulin[5], E. Molinari[2,1], C. Milne[5], F. Boscherini[6,7], and P. Luches[1]

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Metal oxides exhibit remarkable catalytic properties that make them promising candidates for efficient photoelectrochemical applications. Carrier lifetime and mobility play a key role in determining their catalytic performance, making it crucial to investigate the ultrafast electronic and structural dynamics induced by photoexcitation. In CeO_2, functionality relies on the reversible exchange of oxygen ions with reactants, and the formation of photoinduced polarons can enhance reducibility and photocatalytic activity. The associated structural distortions may further lower the oxygen vacancy formation energy, improving redox functionality. A recent pump-probe optical spectroscopy study revealed an ultrafast blue shift in photoinduced absorption by 0.4 eV, attributed to the formation of small polarons within 330 fs from the excitation [1]. This study examines the dynamic evolution of the electronic and crystal structure in stoichiometric CeO_2 films following photoexcitation, employing free-electron laser-based pump-probe X-ray absorption spectroscopy at the Ce L_3 edge in both the near-edge (XANES) and extended energy (EXAFS) ranges. The analysis of the differential pump probe spectra in the XANES region (Fig. 1a) and of the dynamic evolution of the signal intensity (Fig. 1b) revealed that in the first few tens of fs the electronic structure undergoes modifications that are compatible with a transient occupation of Ce 4f states. Within » 500 fs, the electronic structure partially relaxes to a metastable photoexcited state. This partial relaxation is accompanied by a simultaneous structural expansion of about 0.1 Å in the first shell of O atoms around the excited Ce ion as determined by the analysis of pump-probe spectra in the EXAFS region (Fig. 1c), reinforcing the hypothesis of formation of a photoinduced polaronic state. The electronic and structural modifications persist for more than 300 ps.

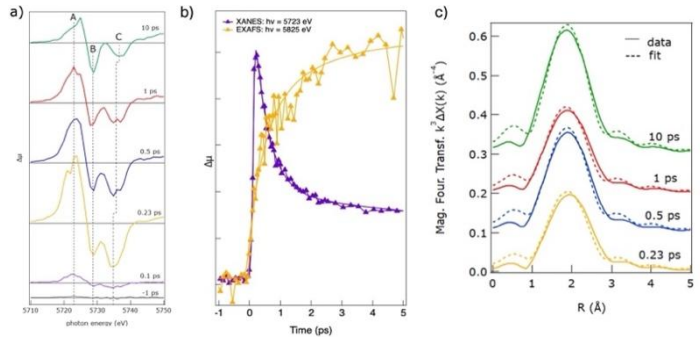

Fig. 1: a) Ce L_3-edge XANES pump-probe difference spectra at different delay times; b) Kinetic traces of the Ce L_3 edge pump-probe signal in the XANES region at hn=5723 eV (purple) and in the EXAFS region at hn=5825 eV (yellow), with the exponential fits of the signals in the 0-5 ps region; c) Magnitude of the Fourier transform of the k^3-weighted first-shell $D\chi(k)$ (solid lines) and fits (dashed lines) at different delay times.

Reference

[1] J. S. Pelli Cresi, L. Di Mario, D. Catone, F. Martelli, A. Paladini, S. Turchini, S. D'Addato, P. Luches, and P. O'Keeffe. *Ultrafast Formation of Small Polarons and the Optical Gap in CeO_2.* J. Phys. Chem. Lett. 11, 5686 (2020).

[O1.08] Advancing Quantum Computing with Quantum Thermodynamics (and vice-versa)

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Quantum thermodynamics studies the (non-equilibrium) thermodynamics of systems and devices operating in the quantum regime. It is a fast-growing field at the cross-roads of thermodynamics, quantum theory, statistical physics, quantum information and quantum technology. Our research activity at Cnr Nano is inspired by the idea that quantum thermodynamics and quantum computing can mutually benefit from each other: On one hand quantum computers offer an unprecedented new experimental tool to put to quantum thermodynamics theory to test, while on the other the latter can be used to improve quantum computing performances. Refs. [1,2] demonstrates the employment of quantum computers to test quantum fluctuation theorems, which are central result of quantum thermodynamics theory. Refs. [3-5] demonstrates the employment quantum thermodynamics methods to prepare high fidelity qubit states on quantum computers, which is crucial for their advancement.

References

[1] A. Solfanelli, A. Santini, and M. Campisi. *Experimental verification of fluctuation theorems with a quantum computer.* PRX Quantum 2, 030353 (2021).

[2] L. Bassman Oftelie and M. Campisi. *Measurement of the work statistics of an open quantum system using a quantum computer.* Quantum Science and Technology, in press (2025).

[3] L. Bassman Oftelie, A. De Pasquale, and M. Campisi. *Dynamic Cooling on Contemporary Quantum Computers.* PRX Quantum 5, 030309 (2024).

[4] L. Buffoni and M. Campisi. *Cooperative quantum information erasure.* Quantum 7, 961 (2023).

[5] L. Buffoni and M. Campisi. *Collective preparation of large quantum registers with high fidelity.* arXiv:2406.16706 (2024).

[O1.09] Optomechanical Metasurfaces

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Metasurfaces have emerged in the last decade as a powerful platform for manipulating waves in unconventional ways, hardly attainable in ordinary materials. Research efforts have targeted both electromagnetic and mechanical waves, as well as the interplay between them, within the framework of *optomechanics*. Here I will review three main activities, summarized by the panels (a)-(c) in Fig. 1.

Fig. 1(a) represents a metal-dielectric-metal metasurface, patterned with chiral L-shaped holes, that has been investigated by means of the *coherent absorption* technique to reveal the singular value and singular vector structure of the scattering matrix. Interesting relations between the sample asymmetry and the S-matrix SVD have emerged, with insights for chiral sensing and polarization manipulation [1,2].

Fig. 1(b) illustrates a metasurface fabricated out of a piezoelectric material, that allows for the excitation of high-frequency (GHz) mechanical Bloch modes. Meanwhile, the metasurface is also resonantly responsive to the optical field, that is eventually modulated. This fully dielectric modulator could prove useful in high-intensity laser beam handling thanks to the absence of any metallic component within the beam path [3,4].

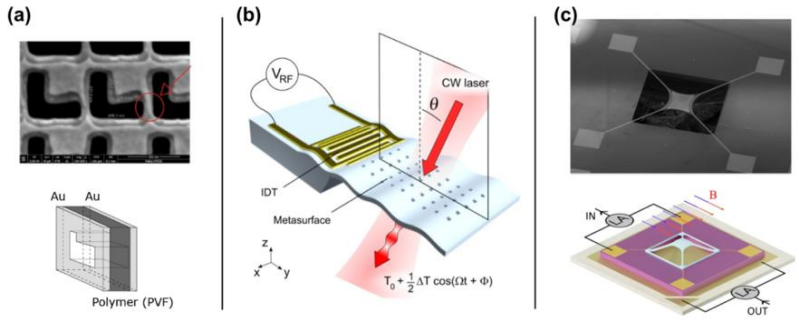

Fig. 1 (a): anisotropic metasurface for studies on the singular value decomposition of the scattering matrix in chiral systems; (b) piezoelectric metasurface for high frequency modulation of laser beams; (c) microbolometric membranes for room-temperature terahertz radiation detectors.

Fig. 1 (c): displays a "trampoline" membrane, that naturally oscillates with sub-MHz frequency; thanks to thermo-mechanical effects, the resonance frequency is sensitive to the energy deposited by incident radiation also in the terahertz (THz) range. Such THz bolometer can be interrogated with a fully electrical scheme based on a magnetoinductive scheme eventually enabling room-temperature operation and multipixel operation [5].

References

[1] S. Zanotto et al. *Photonic bands, superchirality, and inverse design of a chiral minimal metasurface.* Nanophotonics 8 (12), 2291–2301 (2019).

[2] G. Carotta. *Two-sided metal-dielectric-metal devices for light transmission and absorption control*. Thesis to be discussed at University of Pisa (2025).

[3] S. Zanotto et al. *Metamaterial-enabled asymmetric negative refraction of GHz mechanical waves.* Nature Communications 13 (1), 5939. (2022).

[4] A. Pitanti et al. *Gigahertz Modulation of a Fully Dielectric Nonlocal Metasurface.* Advanced Optical Materials 12 (36) (2024).

[5] L. Alborghetti et al. *Enhanced sensitivity of sub-THz thermomechanical bolometers exploiting vibrational nonlinearity.* Submitted.

[O1.10] Coherent coupling between magnons and microwave photons in planar magnet/superconductor hybrid systems

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The coherent coupling between spin wave excitations (magnons) in low-damping magnetic materials and microwave photons has been widely investigated for several possible applications in magnonics and quantum technologies, such as computation, sensing, microwave-to-optical transduction, remote quantum state transfer, emission of microwaves. In recent times, research in this field has been focused on the exploitation of nonlinear effects, either by harnessing the intrinsic nonlinearity of the magnetic system or by integrating it into a superconducting circuit. Another fundamental open point concerns the physical description of the hybrid magnon-photon system in the ultrastrong coupling regime. Current experimental efforts are aimed at finding the appropriate conditions to verify the predictions of general models of light-matter interaction, especially to observe novel phenomena such as the superradiant phase transition.
Here, we present the prototypical case of a bilayer stack realized with an insulating Yttrium Iron Garnet (YIG) film and a high-temperature superconducting YBCO coplanar waveguide (Fig. 1). We report the evolution of magnon and polaritonic spectra detected using broadband lines and resonators, varying the geometry of the experiment and the thickness of the YIG film [1,2]. In particular, we relate the temperature dependence of the characteristic frequencies of the hybrid system, acquired in a wide range between 2 K and 90 K, to the evolution of the penetration depth of YBCO [3]. We demonstrate that the shift of the hybrid mode frequencies can be reproduced by considering the effects of the interaction between spin waves and Meissner currents in the superconductor. Under the optimized conditions, we have obtained collective magnon-photon coupling strengths of 2 GHz, which amounts to 0.2 times the cavity frequency, thus demonstrating the achievement of the ultrastrong coupling regime [1]. The analysis of polariton spectra based on the Hopfield model shows a vanishingly small contribution of the diamagnetic coupling term, which follows as a peculiarity of pure spin systems as in the case of Fe^{3+} magnetic moments in YIG having null orbital contribution. We discuss further experiments for the observation of the superradiant phase transition.

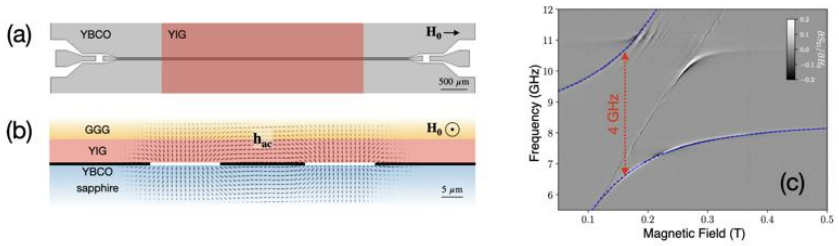

Fig. 1: (a) Top view and (b) section of the YBCO coplanar resonator with the YIG film placed on top. (c) Polariton spectrum acquired at 30 K.

References

[1] A. Ghirri, et al. *Ultrastrong Magnon-Photon Coupling Achieved by Magnetic Films in Contact with Superconducting Resonators.* Phys. Rev. Appl. 20, 024039 (2023).

[2] A. Ghirri, M. Cavani, C. Bonizzoni, and M. Affronte. *Coherent coupling of YBCO superconducting resonators and 100-nm-thick YIG films.* Submitted (2025).

[3] A. Ghirri, C. Bonizzoni, M. Maksutoglu, and M. Affronte. *Interplay between magnetism and superconductivity in a hybrid magnon-photon bilayer system.* Phys. Rev. Appl. 22, 034004 (2024).

[O2.01] Density functional theory of magnetism

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Nearly one hundred years after Heisenberg proposed the first quantum mechanical explanation of ferromagnetism, magnetism continues to pose a challenge for *ab initio* electronic structure theory. The popularity of Density Functional Theory (DFT) in computational materials science is supported by the possibility of improving the involved approximations towards more favorable balance between accuracy and computational effort. The Strongly Constrained and Appropriately Normed (SCAN) density functional represents an important example of a modern approximation of useful wide applicability [1]. But SCAN does not improve the description of magnetism [2].

In this talk, I will show that tackling magnetism via DFT requires: (i) switching from DFT to Spin-Current-DFT [3]; (ii) deriving novel building blocks for U(1)×SU(2) gauge invariant approximations [4]; (iii) extending the generalized Kohn-Sham (GKS) approach to Spin-Current-DFT [5]; and (iv) extending the electron localization function — a widely adopted indicator of bonds and atomic shells — to noncollinear open-shell states [6]. As a result, an improved SCAN for time-reversal spin-orbit-coupled states, ferromagnetic, antiferromagnetic, and noncollinear spin-polarized states is obtained [7,8].

References

[1] J. Sun, A. Ruzsinszky, and J. P. Perdew. *Strongly Constrained and Appropriately Normed Semilocal Density Functional*. Phys. Rev. Lett. 115, 036402 (2015).

[2] F. Tran, G. Baudesson, J. Carrete, G. K. H. Madsen, P. Blaha, K. Schwarz, and D. J. Singh. *Shortcomings of meta-GGA functionals when describing magnetism*. Phys. Rev. B 102, 024407 (2020).

[3] G. Vignale and M. Rasolt. *Current- and spin-density-functional theory for inhomogeneous electronic systems in strong magnetic fields*. Phys. Rev. B 37, 10685 (1988). K. Bencheikh. *Spin–orbit coupling in the spin-current-density-functional theory.* J. Phys. A 36, 11929 (2003).

[4] S. Pittalis, G. Vignale, and F. G. Eich. *U(1)×SU(2) gauge invariance made simple for density functional approximations*. Phys. Rev. B 96, 035141 (2017).

[5] J. K. Desmarais, G. Ambrogio, G. Vignale, A. Erba, and S. Pittalis. *Generalized Kohn-Sham approach for the electronic band structure of spin-orbit coupled materials*. Phys. Rev. Materials 8, 013802 (2024).

[6] J. K. Desmarais, G. Vignale, K. Bencheikh, A. Erba, and S. Pittalis. *Electron Localization Function for Noncollinear Spins.* Phys. Rev. Lett. 133, 136401 (2024).

[7] J. K. Desmarais, J. Maul, B. Civalleri, A. Erba, G. Vignale, and S. Pittalis. *Spin Currents via the Gauge Principle for Meta-Generalized Gradient Exchange-Correlation Functionals*. Phys. Rev. Lett. 132, 256401 (2024).

[8] J. K. Desmarais, A. Erba, G. Vignale, and S. Pittalis. *Meta-Generalized Gradient Approximation Made Magnetic.* Phys. Rev. Lett. 134, 106402 (2025).

[O2.02] Structure, electronic and plasmonic properties of amorphous transparent conducting oxide films for plasmonics in the mid-IR

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Transparent conductive oxides like Al-doped ZnO (AZO) and Indium-tin oxide (ITO) are a class of materials that combine high transparency and low resistivity. Additionally, they show an interesting tunable plasmonic response in the near infrared range with an epsilon-near-zero behavior [1]. When conducting films are grown amorphous, they can overcome poor CMOS compatibility, discontinuity, and poor mechanical stability typical of noble metals. The intrinsic absence of grain boundaries allows for the growth of extremely thin smoother films with improved electronic and transport properties. Even though amorphous conductors are known, a theoretical and experimental understanding of the influence of structural disorder on the electronic and optical properties of the films is completely missing.
We have performed DFT calculations that predict electronic modifications with broadening of the valence and conduction edges due to amorphization and symmetry breaking (Fig. 1a) [2]. We have then grown amorphous AZO films by RF magnetron sputtering by increasing Ar pressure and characterized their electronic, electric, and optical properties (Fig. 1b-d). By combining different experimental techniques (XRD, TEM, HAXPES, Hall measurements, FTIR), we have confirmed the electronic properties predicted by DFT and we have correlated them with electrical and optical response. Within this PRIN 2022 project we are going to correlate these properties with the plasmonic response of the system for application in the MID-IR range.

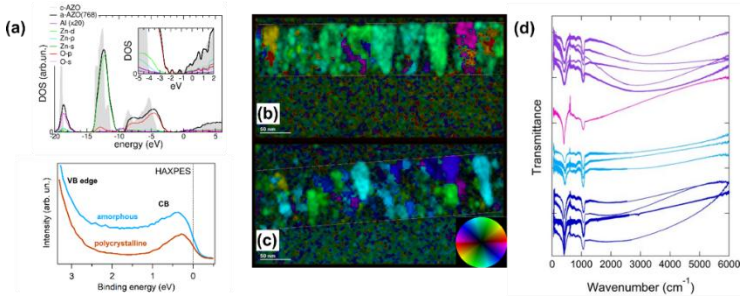

Fig. 1: (a) DFT calculation of DOS and HAXPES measurements on polycrystalline (c-) and amorphous (a-) AZO films; (b,c) FFT analysis of HRTEM images and (d) reflectivity of c- and a-AZO films.

References
[1] G. V. Naik et al. *Alternative Plasmonic Materials: Beyond Gold and Silver*. Adv. Mater. 25, 3264 (2013).
[2] D. Mora-Fonz and A. L. Shluger. *Modeling of Intrinsic Electron and Hole Trapping in Crystalline and Amorphous ZnO*. Adv. Elec. Mater. 6, 1900760 (2020).
[3] R. Magrin Maffei et al. *Defectivity of Al:ZnO thin films with different crystalline order probed by Positron Annihilation Spectroscopy.* Appl. Surf. Sci. 665, 160240 (2024).

Project
NextGeneration EU PRIN 2022 AMONIX – CUP B53D23004060006.

[O2.03] Innovative Polymeric Nanosystems for Drug Delivery Across the Blood-Brain Barrier

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Nanostructured drug delivery systems represent a promising strategy to overcome the challenges associated with therapeutics based on biological macromolecules, particularly in neurodegenerative disorders, where the blood-brain barrier (BBB) severely limits drug access to the central nervous system (CNS) [1]. Our research group has developed innovative polymeric nanocarriers to enhance drug transport across the BBB, focusing on poly(lactide-co-glycolide) (PLGA) nanoparticles (NPs) and stabilized reverse micelles (SRMs).

PLGA NPs are an emerging, biocompatible platform for CNS-targeted drug delivery. By functionalizing their surface with brain-targeting peptides (e.g., Angiopep-2, g7, or Tf2; Fig. 1), we have demonstrated their ability to improve BBB penetration and facilitate lysosomal targeting [2]. As a proof of concept, we applied this approach to Krabbe disease (KD), a lysosomal storage disorder caused by a deficiency of the GALC enzyme. Intravenous administration of NPs loaded with cross-linked enzyme aggregates (CLEAs) of GALC successfully restored enzymatic activity in KD cellular models and in the Twitcher (TWI) mouse, a widely used model of the disease.

To explore alternative, non-invasive drug delivery strategies, we have developed and patented a novel nanostructured platform based on stabilized reverse micelles (SRMs) ["Reversed Micelles for Delivery of Hydrophilic Drugs", ref. 102022000014791]. SRMs are polymeric nanocarriers specifically designed to encapsulate hydrophilic biomolecules while preserving their stability and bioactivity [3].

Using advanced nano-biophysical strategies, such as phasor-based Fluorescence Lifetime Imaging Microscopy (FLIM) [4] via two-photon microscopy and confocal microscopy colocalization analysis, we gained insights into SRMs' internalization, intracellular trafficking, and lysosomal delivery in KD living cells. These studies also revealed their potential role in modulating autophagy, a key cellular pathway disrupted in KD. When administered intranasally, SRMs provide a minimally invasive, patient-friendly approach for CNS drug delivery, leveraging their mucoadhesive properties and ability to cross the BBB to offer an efficient and translationally relevant therapeutic strategy.

Overall, these studies support the effectiveness of integrating advanced nanotechnologies in drug delivery, paving the way for the development of next-generation therapeutics, with considerable potential for enzyme replacement therapies and other targeted treatments for CNS disorders.

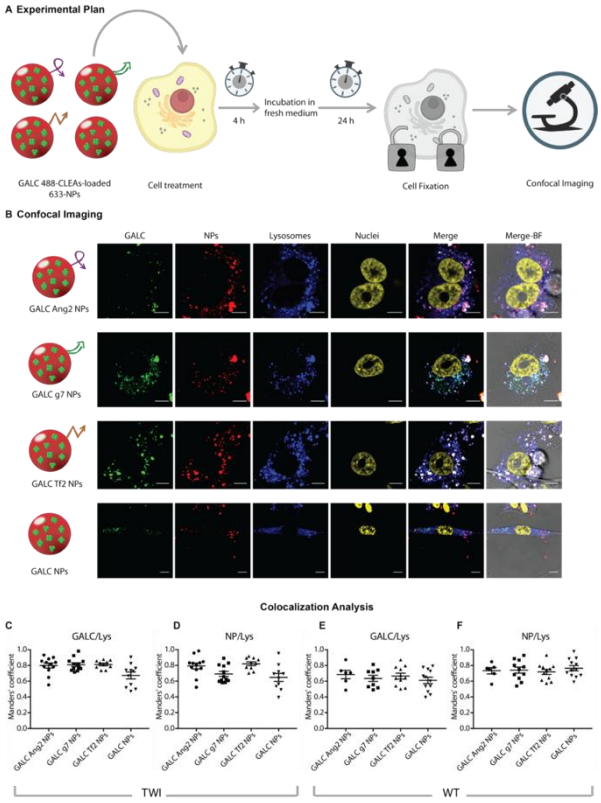

Fig. 1: Intracellular localization of targeted GALC CLEA NPs. (A) Graphical summary of the experiment. Twitcher (TWI) or wild type (WT) primary fibroblasts were incubated with fluorescently labelled GALC CLEA NPs for 4 hours, then washed and added with fresh medium. After 24 h, cell lysosomes were stained, and cells were fixed and imaged with a confocal microscope. (B) Confocal imaging. Representative confocal images of TWI fibroblasts treated with fluorescently labelled GALC Ang2 NPs, GALC g7 NPs, GALC Tf2 NPs or GALC NPs. From the left to the right column: GALC (green, stained with Atto-488), NPs (red, stained with Atto-633), lysosomes (blue, stained with Lysotrack red DND-99), nuclei (yellow, stained with DAPI), superimposition of GALC, NPs, lysosomes and nuclei fluorescence and superimposition of all channels with brightfield image. Scale bars: 10 µM. (C-D) Colocalization analysis. Manders' coefficient of GALC/lysosomes and NPs/lysosomes overlap in TWI cells treated with GALC CLEA NPs. (E-F) Manders' coefficient of GALC/lysosomes and NPs/lysosomes overlap in WT cells treated with GALC CLEA NPs.

References

[1] A. Del Grosso, G. Parlanti, R. Mezzena, and M. Cecchini. *Current treatment options and novel nanotechnology-driven enzyme replacement strategies for lysosomal storage disorders.* Advanced Drug Delivery Reviews 188, 114464 (2022).

[2] A. Del Grosso, M. Galliani, L. Angella, M. Santi, I. Tonazzini, G. Parlanti, and M. Cecchini. *Brain-targeted enzyme-loaded nanoparticles: A breach through the blood-brain barrier for enzyme replacement therapy in Krabbe disease.* Science Advances 5(11), eaax7462 (2019).

[3] M. Gagliardi, A. Vincenzi, L. Baroncelli, and M. Cecchini. *Stabilized Reversed Polymeric Micelles as Nanovector for Hydrophilic Compounds.* Polymers 15 (4), 946 (2023).

[4] V. De Lorenzi, S. Ghignoli, M. Bernardi, G. Matteoli, G. Ferri, B. Storti, R. Bizzarri, and F. Cardarelli. *Measuring pH in insulin secretory granules by phasor-based fluorescence lifetime imaging of a genetically encoded sensor.* Communications Biology. 8 (1), 304 (2025).

[5] A. Del Grosso, L. Angella, I. Tonazzini, A. Moscardini, N. Giordano, M. Caleo, and M. Cecchini. *Dysregulated autophagy as a new aspect of the molecular pathogenesis of Krabbe disease.* Neurobiology of Disease 129, 195-207 (2019).

Project

The SRM-related activities are part of the REMEDY project (“Stabilized REversed MicellEs for brain Delivery of hYdrophilic drugs”), funded by MUR-FISA (CUP: B53C24000900001).

[O2.04] Light-based additive manufacturing for the management of complex fluids

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Additive Manufacturing (AM) methods have gained increasing attention, offering numerous benefits across a wide range of scientific applications. AM is capable of generating3D object in a layer-by-layer fashion, starting from a 3D computer-aided design (CAD) model. Post-processing treatments can also be applied to enhance the physical properties and surface roughness of the printed objects.

While various AM approaches have been introduced to the market, vat photopolymerization is widely employed for manufacturing complex structures with advanced physical properties by polymerizing a pre-polymer by either UV or near-infrared light. A broad range of photo-curable materials have been developed for fabricating objects with high spatial resolution. These capabilities have a significant impact and potential in various fields, including biomaterials, biomedicine, optics and photonics, and droplet microfluidic fabrication [1,2]. In this presentation, we will review the ongoing activities in our group aimed at thethe fabrication of microfluidic devices by digital light processing (DLP) for the generation and analysis of droplet emulsions (Fig. 1). The manufactured devices can generate droplets with varied functionality and high throughput [3-5].

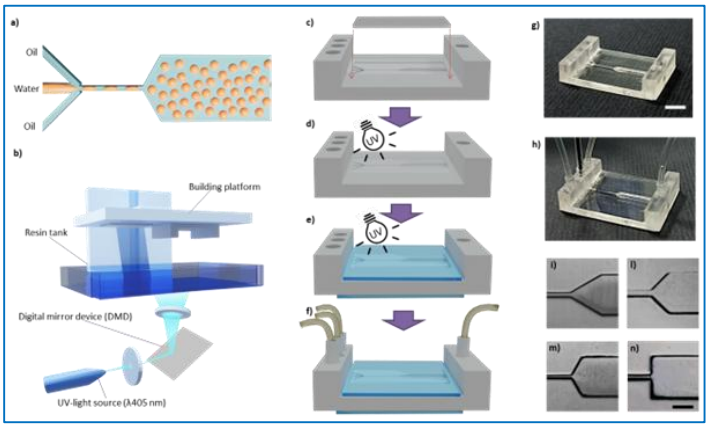

Fig. 1: Schematic representation of a typical geometry for the generation of W/O droplets emulsion. b) Sketch of the DLP 3D printing system. c)-f) Illustration of fabrication steps of a microfluidic device. First, the device with open channels and the sealing layer are printed (c) and bonded through UV-light irradiation (d). Afterwards, two glass coverslips are bonded on the top and bottom surfaces of the device by UV light irradiation and photopolymerization of an interposed layer of pre-polymer (e). Finally, plastic tubes are connected to the inlets and outlet apertures by means of 3D printed connectors (f). g-h) Photographs of the device after step d), (g), and of the final device (h). Scale bars: 9 mm. i-l) Bright field optical microscope images of the inlet of the expansion chamber with opening angle: 30 (i), 45 (j), 60 (k) and 90 (l) degrees. Scale bar: 1 mm. Reproduced from [2].

References

[1] A. Camposeo, et al. Adv. Optical Mater. 7, 1800419 (2019).
[2] S. Orsini, et al. Appl. Phys. Rev. 12, 011306 (2025).
[3] M. Durve, et al. EurPhys J E Soft Matter. 46, 32 (2023).
[4] M. Durve, et al. Physics Fluids 36, 022105 (2024).
[5] M. Durve, et al. *Minimal droplet shape representation in experimental microfluidics using Fourier series and autoencoders.* Physics Fluids 36, 112005 (2024).

Project

The research has received funding from the European Union – Next Generation EU, Mission 4 Component 2 Inv. 1.5 CUP I53C22000780001 and B83C22003930001 (Tuscany Health Ecosystem, Spoke 4: Nanotechnologies for diagnosis and therapy)".

[O2.05] Bridging the Gap: translating Quantum Research into commercial innovation

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The translation of cutting-edge scientific research into commercial innovation is a key challenge in the field of quantum technologies. DSQM S.r.l., a spin-off of the Consiglio Nazionale delle Ricerche (Cnr), represents a successful model of this transition, leveraging decades of fundamental research on superconductors. DSQM focuses on the development and commercialization of next-generation superconducting and quantum devices, with applications ranging from energy-efficient electronics to quantum computing.

The company capitalizes on breakthrough technologies developed within Cnr and European-funded projects, like SPECTRUM and SUPERGATE, including those under the Horizon 2020 and Horizon Europe frameworks, fostering innovation through a synergy between academia and industry. This approach not only enhances European technological sovereignty but also accelerates the adoption of sustainable and energy-efficient materials in strategic sectors.

We will showcase DSQM's technological advancements, its pathway from laboratory discoveries to industrial applications, and the role of European collaborations in fostering high-impact innovation. We will also discuss the challenges and opportunities in bridging the gap between fundamental research and commercial exploitation in the rapidly evolving landscape of quantum materials.

[O2.06] Ultrafast Electron Dynamics in molecules, crystals, interfaces

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I will report on recent advances about ultrafast dynamical phenomena such as photo-injection and photo-induced charge separation and recombination, in materials ranging from covalently bond organic molecules to hybrid heterojunctions and bulk crystals [1-4]. The role of electron-nuclei interaction in triggering the steps of charge injection, delocalization and transfer will be discussed as well as the effect of non-radiative de-excitation channels. The results of first-principles computer simulations, performed by combining Time-dependent Density-Functional Theory and Non-Adiabatic Molecular Dynamics, will be illustrated in conjunction with the results of observations performed with high time resolution pump-probe and 2D spectroscopies. I will finally discuss the scope of the theoretical methods employed and the possible exploitation of the findings in order to design novel materials for photovoltaic and nano-optic applications.

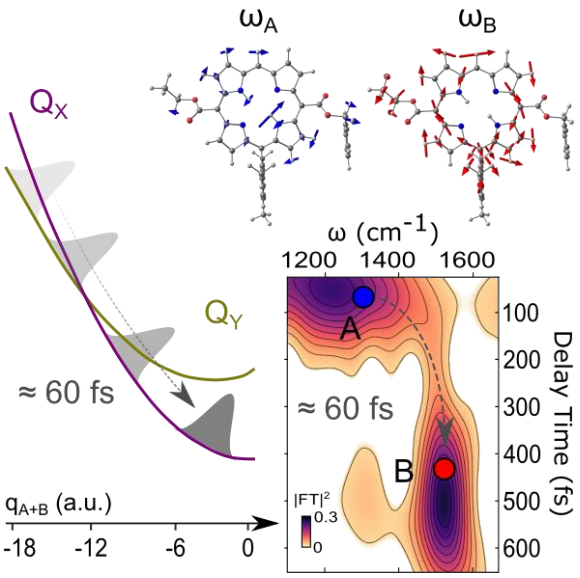

Fig. 1: Internal conversion in a porphyrin derivative proceeds through a crossing of the two Q sub-bands. The vibration modes driving the conversion are theoretically predicted and the ultrafast conversion dynamics is observed via 2D electronic spectroscopy. (from [3]).

References

[1] G. Inzani, et al. *Field-driven attosecond charge dynamics in germanium*. Nat. Photon. 17, 1059 (2023).

[2] A. Casotto, P. S. Rukin, E. Fresch, D. Prezzi, S. Freddi, L. Sangaletti, C. A. Rozzi, E. Collini, and S. Pagliara. *Coherent Vibrations Promote Charge-Transfer across a Graphene-Based Interface.* J. Am. Chem. Soc. 146, 14989 (2024).

[3] V. V. Petropoulos, et al. *Vibronic Coupling Drives the Ultrafast Internal Conversion in a Functionalized Free-Base Porphyrin*. J. Phys. Chem Lett. 15, 4461 (2024).

[4] P. S. Rukin, M. Fortino, D. Prezzi, and C. A. Rozzi. *Complementing Adiabatic and Nonadiabatic Methods To Understand Internal Conversion Dynamics in Porphyrin Derivatives.* J. Chem. Theo. Comput. 20, 10795 (2024).

[O2.07] On-demand Hamiltonians in twisted graphene devices

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2D materials offer an immense toolbox for engineering emergent electronic properties. Specifically, on-demand Hamiltonian design can be achieved by acting on the twist angle between consecutive layers. We have developed techniques to extend this paradigm to CVD graphene crystals, including both monolithically grown and artificially assembled multilayers. These structures allow to control the interlayer hopping [1], introduce superlattices [2], break relevant symmetries [3]. We will especially focus on recent results on structurally asymmetric twisted trilayer graphene, featuring a spontaneous gap opening [3] (see Fig. 1).

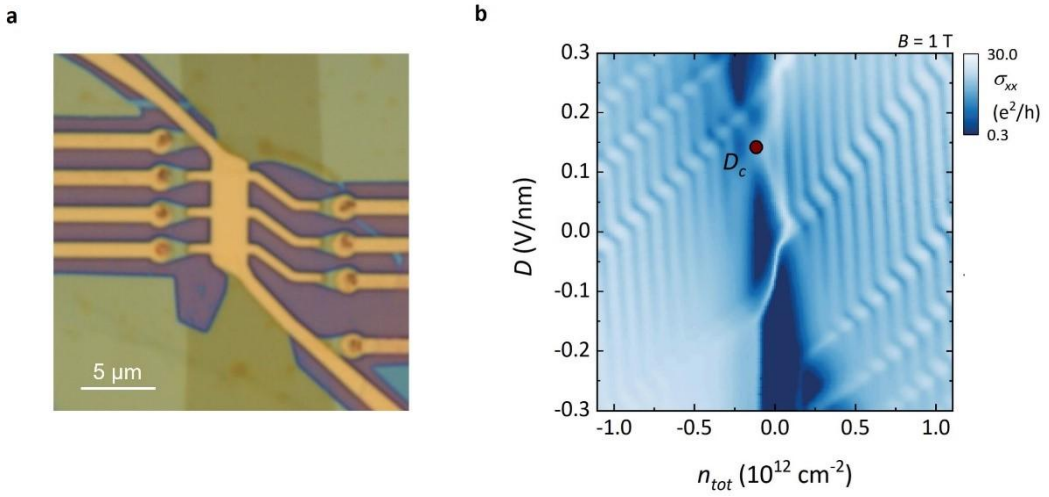

Fig. 1: (a) Optical microscopy image of a dual-gated twisted trilayer device. (b) Longitudinal conductivity at B = 1 T, as a function of charge density (n) and displacement field (D). D_c marks the gap closing in the Bernal subsystem.

References

[1] S. Pezzini, V. Miseikis, G. Piccinini, S. Forti, S. Pace, R. Engelke, F. Rossella, K. Watanabe, T. Taniguchi, P. Kim, and C. Coletti. *30°-twisted bilayer graphene quasicrystals from chemical vapor deposition.* Nano Letters 20, 3313-3319 (2020).

[2] G. Piccinini, V. Mišeikis, P. Novelli, K. Watanabe, T. Taniguchi, M. Polini, C. Coletti, and S. Pezzini. *Moiré-Induced transport in CVD-based small-angle twisted bilayer graphene.* Nano Letters 22, 5252-5259 (2022).

[3] A. Boschi, Z. M. Gebeyehu, S. Slizovskiy, V. Mišeikis, S. Forti, A. Rossi, K. Watanabe, T. Taniguchi, F. Beltram, V. I. Fal'ko, C. Coletti, and S. Pezzini. *Built-in Bernal gap in large-angle-twisted monolayer-bilayer graphene.* Communications Physics 7, 391 (2024).

[O2.08] Terahertz non-linear optics in van der Waals metamaterials: a bridge in the 24-60 um gap

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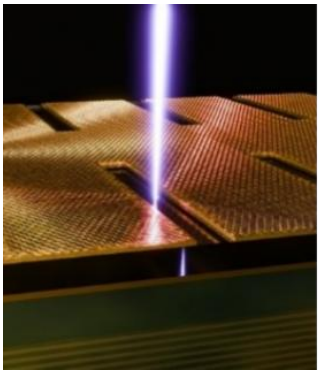
Optical nonlinearity in the terahertz (THz) range represents a key technology to access high frequency spectral windows that are usually difficult to cover using conventional solid state laser technologies. Over the past decade, the non-linear optical properties of graphene have been extensively investigated, and a wide range of related applications demonstrated, ranging from optical modulators [1] to saturable absorbers [2]. High harmonic generation (HHG) – the frequency up-conversion of an optical signal – in materials systems is governed by symmetries. This effect has been exploited in graphene [3], where HHG has been demonstrated, albeit only at odd multiples of the driving frequency owing to its inherent centro-symmetry. In topological insulators (TIs), unconventional HHG has been predicted [4], supported by the bulk and topological surface states, which are usually difficult to distinguish, relying on the ultrafast intraband dynamics, and the inversion symmetry-breaking even-order nonlinearity in the topological phase.

Here, we exploit innovative technological approaches in multilayer graphene or large area TI metametarials and heterostructures, to devise highly efficient non-linear micro-devices and electrically driven plasmonic lasers, targeting HHG in the technologically relevant *Reststrahlen* gap (6-12 THz) at both odd or even orders [5-7]. This talk will provide future perspectives in the fascinating field of topological photonics and non-linear THz photonics.



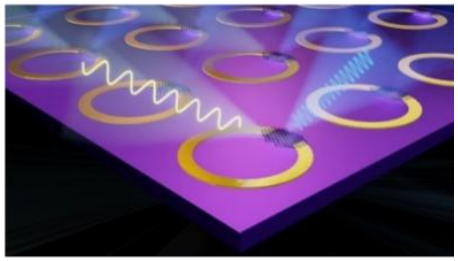


Fig. 1: (a) Schematic diagram of a QCL-pumped graphene split ring resonator array: pumped light is frequency upconverted at the third harmonic frequency. (b) Device schematics of a plasmonic heterostructure laser with an integrated topological insulator stack.

References

[1] A. Di Gaspare, et al. *Electrically Tunable Nonlinearity at 3.2 Terahertz in Single-Layer Graphene*. ACS Photonics 10, 3171−3180 (2023).

[2] A. Di Gaspare, et al. *All in one-chip, electrolyte-gated graphene amplitude modulator, saturable absorber mirror and metrological frequency-tuner in the 2-5 THz range.* Adv. Optical Mater. 10, 2200819 (2024).

[3] H. A. Hafez, et al. *Extremely efficient terahertz high-harmonic generation in graphene by hot Dirac fermions*. Nature 561, 507–511 (2018).

[4] J. Stensberg, et al. *Observation of terahertz second harmonic generation from Dirac surface states in the topological insulator Bi2Se3.* Phys. Rev. B 109, 245112 (2024).

[5] A. Di Gaspare, et al. *Compact terahertz harmonic generation in the Reststrahlenband using a graphene-embedded metallic split ring resonator array.* Nature Commun. 15, 2312 (2024).

[6] A. Di Gaspare, et al. *Second and third harmonic generation in topological insulator-based van der Waals metamaterials*. Nature Light Science&Applications (2025).

[7] A. Di Gaspare, et al. *Electrically-driven heterostructured wire lasers with integrated graphene plasmons*. Under review.

[O2.09] Hole-spin qubits in germanium beyond the single-particle regime

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Spin qubits in semiconductor quantum dots (QDs) are promising candidates for the implementation of scalable quantum computers [1, 2], thanks to well-advanced fabrication techniques and integration circuitry that allow a high degree of control even at relatively high temperatures (up to 4K) [3]. In contrast to electrons, holes in Ge have no valley degeneracy and are characterized by a strong spin-orbit coupling, which allows for all-electric manipulation [4], and are only weakly affected by the hyperfine interaction. Due to these attractive features, hole-spin qubits in germanium quantum dots are at the forefront of quantum computing research.

In this work [5], we study three-hole spin qubits in Ge QDs, implemented in unstrained MOS-like devices and in $Ge/Si_{1-X}Ge_X$ heterostructures, a concept that is still relatively unexplored from the theoretical point of view. This qubit encoding, while being analogous to the single-hole one, is not subjected to the restricting condition of having to reach the last-hole occupation of the QD. Most importantly, we show that the main figures of merit are always at least comparable to those obtained for single holes and are significantly higher in certain confinement regimes. Specifically, the Rabi frequency of the 3-hole qubit is shown to exceed that of the 1-hole qubit by up to 2 orders of magnitude in quasi-circular QDs. Biaxial strain leads to an overall reduction of the Rabi frequencies, which is however compensated by a proportional increase in the inhomogeneous dephasing time. The various scenarios considered in this work consistently point to the fact that three-hole spin qubits in Ge perform better than their single-hole counterparts when the QD is close to the circular regime – an indication for advantageous experimental implementations.

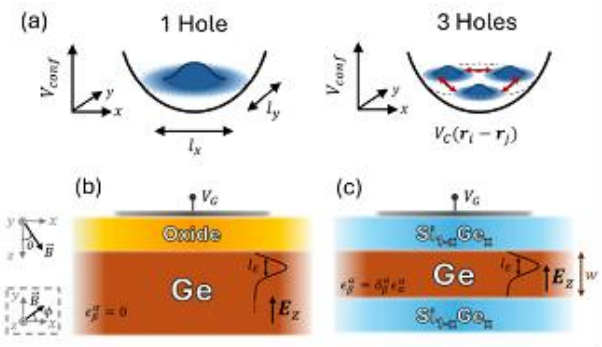

Fig. 1: Scheme of the considered devices.

References

[1] D. Loss and D. P. DiVincenzo. *Quantum computation with quantum dots*. Phys. Rev. A 57, 120 (1998).

[2] G. Scappucci, et al. *The germanium quantum information route*. Nature Reviews Materials 6, 926 (2021).

[3] L. C. Camenzind, et al. *A hole spin qubit in a fin field-effect transistor above 4 kelvin*. Nature Electronics 5, 178 (2022).

[4] L. Bellentani, et al. *Toward hole-spin qubits in Si p-mosfets within a planar cmos foundry technology.* Phys. Rev. Applied 16, 054034 (2021).

[5] A. Secchi, et al. *Hole-spin qubits in germanium beyond the single-particle regime.* In preparation (2025).

[O2.10] Electron particles to control electron waves in graphene systems

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Electron optics explores the wave-like properties of electrons in conductors, applying optics principles to electronic systems. Although the fascinating potentiality in mimicking photonic circuits with solid state devices and their electrons to advance in quantum technologies, sensing and fundamental physics, electron optics still lacks the ideal platform. Graphene has given new life, overcoming the need of the quantum Hall regime like in the historically dominant two-dimensional electron gases. In graphene, the key actors are the *pn* junctions, with which electron-waves interact like electromagnetic waves in dielectrics, thus following optics principles. Although its local control, the standard electrostatic gating to induce *pn* junctions lacks efficiency, high lateral resolution, and flexibility. Thus, optics-like lenses and waveguides have been demonstrated but never coupled together to form electron-optics circuits.

This activity aims to revolutionize electron optics by demonstrating the first all-electron-optical circuits in graphene and their main building blocks. To this scope, I will employ a novel methodology to realize and combine *pn* junctions that focus, collimate, and act as beam splitter to unlock the realization of compact photonics-like electronic circuits, such as integrated Mach-Zehnder interferometers. Specifically, *pn* junctions will be created with unprecedented resolution [1] and control of their profile by deterministically introducing defects in the graphene lattice via low-energy electron-beam irradiation [2]. By these junctions, a Fabry-Pérot interferometer has been recently demonstrated in conditions not achievable by electrostatic gating, that is graphene field-effect transistors with minimum cavity length of about 25 nm [3].

In conclusion, this activity will create a new electronic paradigm by merging the excellence of electronic circuits with that of photonic systems, elevating the electron-optics to a superior level, opening a new roadmap toward unexplored fundamental phenomena in electron-optics.

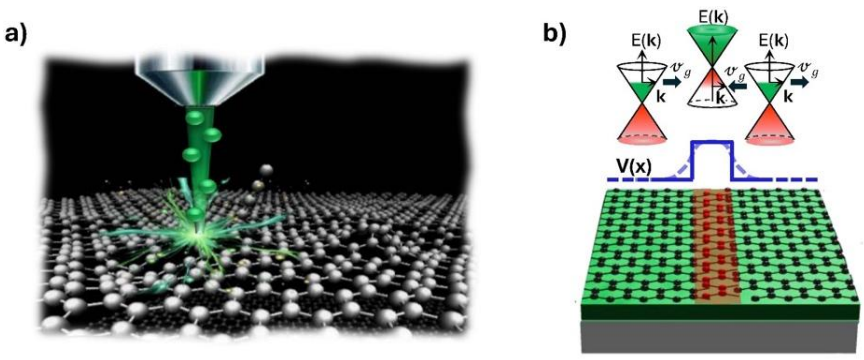

Fig. 1 Main key-actors a) Cartoon describing the electron-irradiation process of graphene sheets. b) (top) Band structure of graphene and the dispersion relation of wavevector (k) and group velocity ($\hbar v_g$) for a *npn* junction and (center) potential profile V(x) in sharp (blue solid line) and smooth condition (light blue dashed line). (bottom) Substrate-supported pristine graphene sheet (green areas and black atoms) containing a defective line (red area and atoms).

References

[1] N. Melchioni, F. Fabbri, A. Tredicucci, and F. Bianco. *Periodic Structural Defects in Graphene Sheets Engineered via Electron Irradiation.* Micromachines 13, 1666 (2022).

[2] N. Melchioni, L. Bellucci, A. Tredicucci, and F. Bianco. *Operability timescale of defect-engineered graphene.* Surf. Interf. 37, 102662 (2023).

[3] N. Melchioni, F. Paolucci, P. Marconcini, M. Macucci, S. Roddaro, A. Tredicucci, and F. Bianco. *Tailoring coherent charge transport in graphene by deterministic defect generation.* arXiv:2409.04858 (2024).

[O2.11] Polymeric Piezoelectrics for Energy Harvesting Applications

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Piezoelectric phenomena rely on the capability of non-centrosymmetric crystalline materials to generate electrical charges on their surface upon mechanical deformations.
Both natural and synthetic piezoelectric polymers and biomolecules can convert mechanical deformation into electrical signals and still maintain their major character in terms of flexibility and robustness, as well as environmental sustainability and biocompatibility. Though they show lower piezoelectric coefficients and electromechanical coupling factors compared to mostly used piezoelectric ceramics, their impact on energy harvesting technologies is increasing. To boost their piezoelectric performance and enable their integration into complex electronic systems, different approaches can be exploited such as chemical processing, micro- and nano-structuring, fabrication of composites with organic/inorganic fillers in polymer matrixes and cooperative networks of electrospun nanofibers [1]. As a result, energy harvesters based on these materials and simple design offer promising prospects for (self-) powering systems, whose applications can range from biomedical engineering and healthcare monitoring to environmental sensing and soft robotics.
Here, we discuss the diverse exploitable strategies to obtain outstanding piezoelectric performances and report on piezoelectric sensors and energy harvesting devices based on composite systems of natural polymeric materials and nanofibers [2,3].

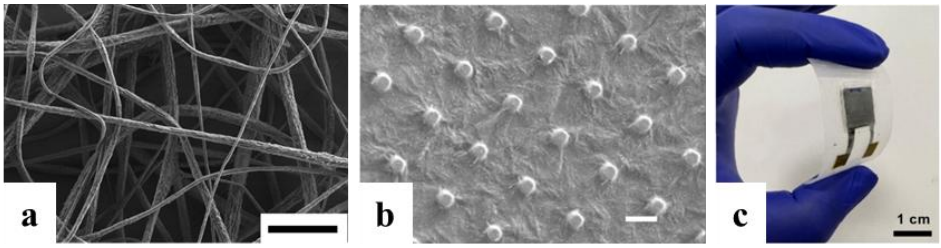

Fig. 1: Scanning electron micrographs of a) random piezoelectric polymer nanofibers (Scale bar: 5 µm) and b) nanopatterned Cellulose/Polyvinyalcohol composite, planar view (Scale bar: 1 µm). c) Photograph of a flexible piezoelectric device.

References

[1] L. Persano, S.K. Ghosh, and D. Pisignano. *Enhancement and Function of the Piezoelectric Effect in Polymer Nanofibers.* Acc. Mater. Res. 3, 900 (2022).
[2] B. Azimi, M. Labardi, M. S. S. Bafqi, T. Macchi, C. Ricci, V. Carnicelli, L. Scarpelli, I. Hussain, F. Matino, M. Scaglione, D. Pisignano, A. Lazzeri, M. J. Uddin, L. Persano, and S. Danti. *Remnant polarization and structural arrangement in P(VDF-TrFE) electrospun fiber meshes affect osteogenic differentiation of human mesenchymal stromal cells.* Materials & Design 241, 112973 (2024).
[3] S. K. Ghosh, F. Matino, F. L. Favrin, I. Tonazzini, R. D'Orsi, J. G. de la Ossa, A. Camposeo, J. Li, W. Liu, T. A. Hacker, D. Pisignano, A. Operamolla, X. Wang, and L. Persano. *Fully biodegradable hierarchically designed high-performance nanocellulose piezo-arrays*. Sci. Adv. 11, eads0778 (2025).

Projects

European Commission's Marie Skłodowska-curie Actions (MScA), through the Marie Skłodowska-Curie Individual Fellowship (896811-BiOiMd and h2020-MScA- iF- 2019) and the European Union by the next Generation EU project "NEST – network 4 energy Sustainable transition" (Pe0000021 and CUP B53c22004060006).

[O2.12] Nano and microengineered chitosan-based scaffolds as a tuneable approach for peripheral nerve regeneration applications

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The use of Chitosan, a natural, biodegradable, and biocompatible material has been highly explored in regenerative medicine in the recent years. In clinics, it is approved to produce supports (scaffolds) for the repair of peripheral nerve injuries (PNIs). PNIs, a condition in which a peripheral nerve is damaged, affect more than one million people every year globally, often having life-altering consequences for patients. Chitosan conduits are now being used to reconnect broken nerves, however, chitosan exploitation in regenerative devices is limited by its brittleness and stiffness. Scaffolds can be further tuned, for example, by blending with other materials, by tuning their superficial microstructure or by functionalizing them.

Here, we modulated some key physical properties of chitosan substrates (superficial topography, stiffness, electrical conductivity, or bioactive functionalization) with the aim to improve their use as scaffolds in nerve regeneration.

Firstly, we developed soft membranes made of chitosan and glycerol (Gly-Chi) and micropatterned with directional geometries (gratings with line width ≈ 5 μm) with different levels of axial symmetry [1]. The glycerol-blended chitosan membranes were optimized in terms of mechanical properties and present a physiological-grade Young's modulus (≈ 0.7 MPa), like the nerve tissue. The membranes were then tested in vitro with Schwann cells (SCs), the glial cells that as first support axonal regeneration and myelination in the PNS, and induced pluripotent stem cells– derived nociceptors (sensory neurons, SN), also in co-cultures. Importantly, Gly-Chi membranes significantly improve the collective migration performance of SCs, compared to pure and stiffer chitosan membranes with same topographies. The nerve-in vitro-model made of primary SCs and SN successfully grew over the Gly-Chi membranes, and the topography played an important role in directing not only the cytoskeletal organization of SCs but also the axonal elongation of the neurons. Finally, Gly-Chi microstructured scaffolds were tested in an *in vivo* model of cavernous nerve injury resembling the damage to the neurovascular bundle that occurs after radical prostatectomy, with promising results. To further enhance the regenerative potential of these soft microstructured membranes, we introduced functional modifications, by tuning their electrical properties or the controlled release of drugs. I) For electrical conductivity, a graphene monolayer was integrated on Gly-Chi membranes via an optimized transfer method and subsequently tested with SCs in vitro. II) As biochemical functionalization, the Gly-Chi membranes were functionalized with Sildenafil, a phosphodiesterase inhibitor drug with well-documented neuroprotective and neuroregenerative properties; Sildenafil was successfully incorporated into the scaffolds, preserving their stability, microstructure, and biocompatibility with SCs, and was also successfully released from the membranes.

Overall, the results highlight the possibility to develop biocompatible chitosan-based microstructured membranes functionalized with functional or biochemical cues as an innovative strategy for improving peripheral nerve regeneration.

Reference

[1] L. Scaccini, R. Mezzena, A. De Masi, M. Gagliardi, G. Gambarotta, M. Cecchini, and I. Tonazzini. *Chitosan Micro-Grooved Membranes with Increased Asymmetry for the Improvement of the Schwann Cell Response in Nerve Regeneration.* Int J Mol Sci. 22, 7901 (2021).

Abstracts | Poster Presentations Day 1 (June 05, 2025)

[P1.01] A controlled sub-cellular mechanical stimulus to study PIEZO2 channel activation

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The mechanosensitive PIEZO2 channel is the main transducer of mechanical stimulus in light touch, proprioception [1], whose alteration is involved in hypersensitivity and pain [2]. While its gating mechanisms are partially understood, the modulation of PIEZO2 by mechanical stimuli remains unclear.
The investigation of PIEZO2 function can greatly benefit from combining nanotechnological tools such as Atomic Force Microscopy (AFM) and Fluidic Force Microscopy (FluidFM) with calcium imaging. AFM and FluidFM are techniques, that stand out for their precision in applying a localized mechanical stimulus on a region of a cell, allow a fine control over the force/pressure intensity, subcellular localization and directionality, which integrated calcium imaging enable to monitor the activity of PIEZO2 mechanosensitive calcium channels.
For this reason, we transfected in HEK-293 cells PIEZO2-green lantern, a chimera protein that enables also to localize the PIEZO2 channels in the cell. By using a bead-modified AFM probe, single PIEZO2-transfected cells were vertically stimulated on the nuclear region (Fig.1A) using 50nN force for short (0.5s) and long (10s) duration. Our results demonstrated that PIEZO2 channels are highly sensitive, with a low activation threshold of 50nN (approximately +10 mmHg), and efficiently respond to short-duration stimuli, aligning with their physiological role in light-touch perception. Notably, PIEZO2 activation triggered a collective calcium response in neighboring cells, suggesting a role in mechanosensitive cell-cell communication.
Mechanical stimulation using a bead-modified cantilever can activate mechanosensitive channels on both the plasma and intracellular membranes. To specifically target plasma membrane channels, we utilized FluidFM. The microchanneled cantilever, connected to a pump system, was brought with a controlled force into contact with the soma of dorsal root ganglion (DRG) cells, which naturally express PIEZO2 (Fig. 1B). This system allowed for the application of localized positive and negative pressure at the plasma membrane, revealing differential localized response depending on culture time, potentially indicating changes in channel expression or in its plasma membrane localization. Moreover, a higher response was generally observed both for a positive and negative pressure of 80 mBar.
This study highlights the potential of AFM and FluidFM in elucidating PIEZO2 functionality and its broader physiological and pathological role. Supported by PRIN 2020 – Project Touch on a Chip.

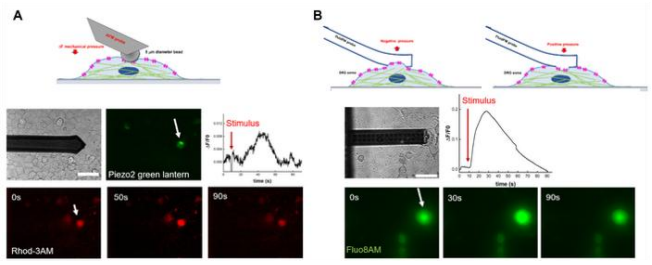

Fig.1: Single cell response upon localized mechanical stimulation (A) Bright-field showing the AFM cantilever in contact with the HEK cells expressing PIEZO2-Green Lantern green in fluorescence image and indicated by white arrow; calcium trace (ΔF/F0) showing the response upon mechanical stimulation (50 nN) applied at the time indicated by the red arrow; lower panel time-lapse images showing Rhod-3AM fluorescence indicating cytosolic calcium at 0, 50, and 90s. (B) Bright field showing the position of the FluidFM cantilever on DRG soma; calcium trace (ΔF/F0) indicating the response upon application of + 40mbar at the time indicated by the red arrow; in the lower panel time-lapse images showing Fluo-8 fluorescence signal at 0, 30, and 90s.

References

[1] S. Ranade, et al. *Piezo2 is the major transducer of mechanical forces for touch sensation in mice.* Nature 516, 121–125 (2014).
[2] R. Syeda. *Physiology and Pathophysiology of Mechanically Activated PIEZO Channels.* Annu. Rev. Neurosci. 44: 383–402 (2021).

[P1.02] A benzodiazepine-derived molecule affects the proliferation and migration of glioblastoma-astrocytoma cells by altering their bio-mechanical properties

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Glioblastoma multiforme (grade IV glioma) is characterized by a high invasive potential making surgical intervention extremely challenging and patient survival very limited. Current pharmacological approaches show at best slight improvements in the therapy against this type of tumour. Here we analysed, on a cellular model of glioblastoma multiforme, the effect of 1-(4-amino-3,5-dimethylphenyl)-3,5-dihydro-7,8-ethylenedioxy-4h2,3-benzodiazepin-4-one molecule (hereafter referred to as 1g) which was shown to act as a cytostatic drug in other cell types by affecting microtubule dynamics. We found that 1g acts also as a migration suppressor by inducing a loss of cell polarity. We characterized the mechanics of U87MG cell aggregates exposed to 1g by different biophysical techniques [1]. We considered both 3D aggregates and 2D cell cultures testing substrates of different stiffness. We established that this molecule produces a decrease of cell spheroid surface tension (Fig. 1), of collective contractility and it impairs 3D cell invasion. At the same time, in the case of isolated cells, 1g selectively produces an almost instantaneous loss of cell polarity blocking migration and it also produces a disorganization of the mitotic spindle when cells reach mitosis. We can state that the studied molecule produces similar effects to other molecules that are known to affect the dynamics of microtubules, but probably indirectly via microtubule-associated proteins (MAPs) and following different biochemical pathways.

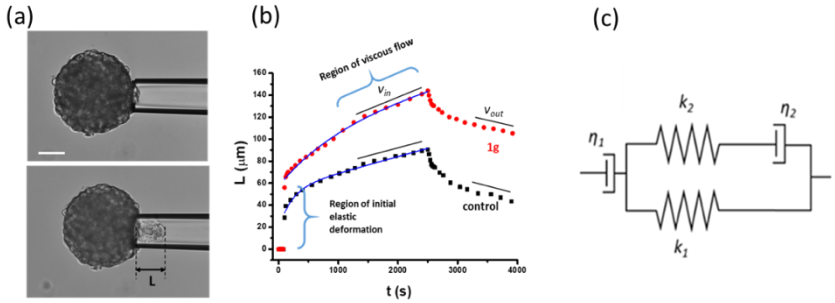

Fig. 1: Micropipette aspiration of U87MG spheroids. (a) Sequence of two images during the aspiration process of an U87MG spheroid exposed to 20 µM 1g. L represents the length of the tongue to be used for the fitting procedure (bar = 50 µm for both images); b) Representative aspiration and relaxation curves for a control spheroid (black squares) and 1g treated spheroid (red circles). The continuous lines represent the fit of the equation representing the creep relaxation; c) Rheological model exploited for the fitting procedure.

Reference

[1] G. Ragazzini, A. Mescola, R. Tassinari, A. Gallerani, C. Zannini, D. Di Rosa, C. Cavallini, M. Marcuzzi, V. Taglioli, B. Bighi, R. Ettari, V. Zappavigna, C. Ventura, A Alessandrini, and L Corsi. *A benzodiazepine-derived molecule interferes with the bio-mechanical properties of glioblastoma-astrocytoma cells altering their proliferation and migration.* Int. J. Mol. Sci, accepted. (2025).

[P1.03] Multiscale modelling of biological effect of ionizing radiation. Investigating the sparing effect of FLASH and minibeam modalities

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Radiotherapy (RT) is one of the primary weapons against cancer, with the main drawback of toxicity for the normal tissues surrounding irradiated areas. In the last decade, evidence was established that temporally as well as spatially bunched radiations can selectively spare normal tissues while keeping at least the same efficacy on the cancerous ones, i.e., through ultrahigh dose rate ("FLASH" RT) or comb shaped (mini/micro beam) irradiation modalities. While the clinical translation of these potentially disruptive new radiotherapy techniques is currently in the starting phase, the underlying mechanism of the differential effects in cancer vs normal tissues are not fully understood. A number of hypotheses is currently under investigation involving, among others, nonlinear effects in radicals production/depletion, detoxify/recover pathways, intra/inter cellular diffusion of toxic substances/recovery signaling, and others, none of which entirely satisfactory [1].

Any of the hypothetical determinant processes involves a cascade of events from the subcellular level up, whose study requires an inherently multi-disciplinary effort. In this talk, we first contextualize the problem and illustrate the general approach used in the modeling group@NANO to study the intrinsically selectivity of FLASH-RT related techniques. This involves the combination of multi-scale (Fig.1) Molecular Dynamics and Monte Carlo simulations with empirical stochastic and kinetic models, and neural network algorithms. We then focus on the optimization of a stochastic minimalist model including the main subcellular features and capable of capturing the differential effects. This approach relies on continuous interactions with experimental groups producing radio-biological data in vitro and in vivo, which we realize within large collaborations with other CNR institutes, UniPi, AoPI, INFN-sezPI and CPFR, supported by PNRR, Fondazione Pisa, INFN, MIUR and EU.

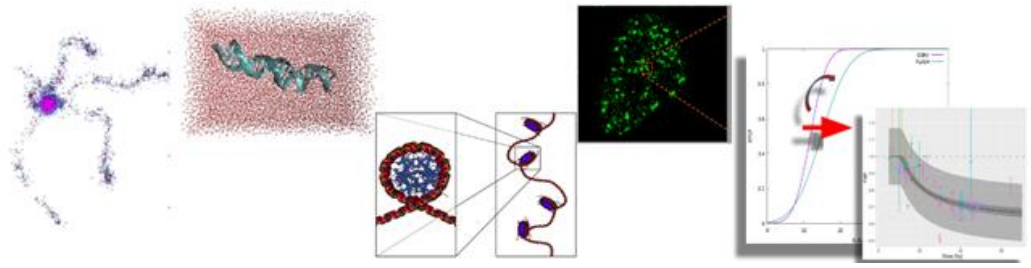

Fig. 1: Multiscale cascade of effects following energy deposition from ionizing radiation (left most panel from Boscolo, et al. IJMS 2020, rightmost panel from [2]).

References

[1] M.-C. Vozenin, B. W. Loo Jr., S. Tantawi, P. G. Maxim, D. R. Spitz, C. Bailat, and C. L. Limoli. *FLASH: New intersection of physics, chemistry, biology, and cancer medicine.* Reviews of Modern Physics 96, 035002 (2024).

[2] T. T. Böhlen, J. F. Germond, J. Bourhis, M.-C. Vozenin, E. M. Ozsahin, F. Bochud, C. Bailat, and R. Moeckli. *Normal Tissue Sparing by FLASH as a Function of Single-Fraction Dose: A Quantitative Analysis.* Int J Radiat Oncol Biol Phys. 114, 1032-1044 (2022).

[P1.04] Exploring GPR65 as therapeutic target in Krabbe disease

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Krabbe disease (KD) is a lysosomal storage disorder caused by a deficiency of galactosylceramidase (GALC). The loss of GALC function results in the accumulation of psychosine (PSY) in the nervous system, leading to demyelination and neurodegeneration. Currently, there is no cure for KD, and the available treatments are primarily supportive [1]. Emerging evidence suggests that correcting GALC deficiency and clearing PSY may not be sufficient to fully restore the KD phenotype [2], implying the involvement of additional, unidentified factors in disease pathogenesis.

In this study, we provide clear evidence supporting the role of G protein-coupled receptor 65 (GPR65) as a key mediator in a PSY-independent mechanism of KD. Our findings demonstrate a significant downregulation of GPR65 in the lymphocytes of KD patients compared to healthy controls (Fig. 1). Similar GPR65 downregulation was observed in the thymus of KD model mice, indicating a novel pathway contributing to disease progression.

These results form the foundation of the project "Study of GPR65 as a New Krabbe Disease Drug Target" funded by the European Leukodystrophy Association (ELA, g.n ELA2023-006C4). The project aims to evaluate the therapeutic potential of GPR65 mRNA-based therapy using brain-targeted nanoparticles, both as a standalone treatment and in combination with GALC correction.

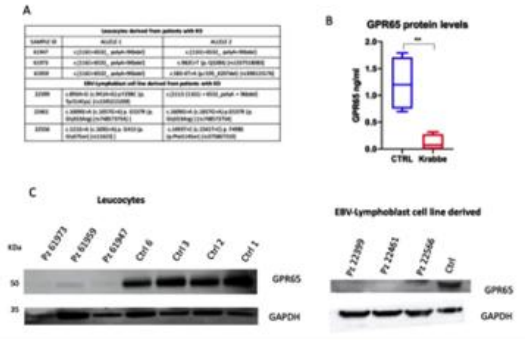

Fig. 1: Decreased expression of GPR65 in immune cells derived from patients with KD compared to healthy subjects. (A) GALC genotype of patients with KD; (B) GPR65 levels in the immune cells from patients with KD and healthy subjects were determined by ELISA ** P < 0,01 Krabbe disease vs healthy subjects, Student's t-test; (C) Western blot analysis of the GPR65 expression.

References

[1] D. A. Wenger, M. A. Rafi, P. Luzi, J. Datto, and E. Costantino-Ceccarini. *Krabbe disease: genetic aspects and progress toward therapy.* Mol. Genet. Metab., 70, 1–9 (2020).

[2] A. M. Bradbury, E. R. Bongarzone, and M. S. Sands. *Krabbe disease: New hope for an old disease*. Neuroscience Letters (2021).

[P1.05] 3D printed magnetically actuated substrates for lung epithelial cell culture

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Additive manufacturing (AM) and 4-dimensional (4D) printing are attracting growing interest since they allow for the fabrication of complex three-dimensional (3D) architectures capable of shape transformation in response to specific stimuli [1]. In tissue engineering, this technology enables the generation of smart biomimetic systems capable of controlled shape transformation in response to certain stimuli, such as heat, light, and electric or magnetic fields. These features make 4D printing a powerful technology for advancing dynamic tissue modeling [2].

Pulmonary diseases are among the leading causes of mortality worldwide; thus, advanced in vitro models that accurately recapitulate lung physiopathology are critical for boosting basic research on pulmonary pathologies as well as drug design and discovery [3]. For this reason, biomimetic 3D models are increasingly replacing standard 2D cultures, yet most do not account for the physical forces to which lung cells are subjected and that impact cell behavior [3].

Here, we introduce the design and characterization of magnetically actuated 3D-printed substrates as a smart biological platform for lung epithelial cell culture. The substrates, fabricated by digital light processing using a photocurable resin doped with magnetic nanoparticles, successfully respond to a static magnetic field. Different functionalization strategies to promote cell attachment and viability have been explored in vitro. Wettability and surface properties were characterized, while biocompatibility assessment confirmed good cytocompatibility and the ability to sustain cell proliferation. These preliminary findings suggest the potential of magnetically actuated functionalized substrates for developing advanced lung modeling platforms.

References

[1] X. Wan, Z. Xiao, Y. Tian, M. Chen, F. Liu, D. Wang, Y. Liu, P.J.D.S. Bartolo, C. Yan, Y. Shi, R. R. Zhao, H. J. Qi, and K. Zhou. *Recent Advances in 4D Printing of Advanced Materials and Structures for Functional Applications.* Advanced Materials 36, 2312263 (2024).

[2] J. Lai, Y. Liu, G. Lu, P. Yung, *et al*. *4D bioprinting of programmed dynamic tissues.* Bioactive Materials 37, 348-377 (2024).

[3] L. Fallert, B. A. Urigoitia-Asua, A. Cipitria, and D. Jimenez de Aberasturi. *Dynamic 3D in vitro lung models: applications of inorganic nanoparticles for model development and characterization.* Nanoscale 16, 10880 (2024).

Projects

European Union – Next Generation EU, Mission 4 Component 2 Inv. 1.5 CUP I53C22000780001 and B83C22003930001 (Tuscany Health Ecosystem, Spoke 4: Nanotechnologies for diagnosis and therapy).

[P1.06] Nanovectors for nose-to-brain delivery of antisense oligonucleotides

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Nanotechnology has revolutionized biomedical research by enabling precise drug delivery, improving therapeutic efficacy, and minimizing systemic side effects. Nanoscale drug carriers offer new opportunities for treating genetic and neurodevelopmental disorders by enhancing bioavailability, enabling targeted distribution, and overcoming biological barriers. However, the blood-brain barrier remains a major challenge, limiting the delivery of therapeutic molecules to the central nervous system (CNS).
Antisense oligonucleotides (ASOs), short synthetic nucleic acid sequences that selectively bind target RNAs to modulate gene expression, have gained attention as potential therapeutic treatments for genetic and neuro-developmental/degenerative disorders, including Angelman syndrome (AS). However, effective ASO delivery to the brain remains a challenge, as current approaches rely on invasive methods like intrathecal injections, which carry a high risk of side effects and poorly understood distribution kinetics. To address this challenge, we are developing nanoparticle (NP)-based systems for intranasal ASO brain delivery. Our approach involves the design and characterization of three distinct biodegradable and mucoadhesive nanocarriers: (i) chitosan nanoparticles crosslinked with 2,6-pyridinedicarboxylic acid [1]; (ii) Poly (D, L–lactide-co-glycolide) (PLGA) nanoparticles with an external mucoadhesive coating; and (iii) stabilized reverse micelles in PLGA for hydrophilic drug encapsulation [2]. Our studies demonstrate that all three NP formulations exhibit optimal physicochemical properties, including controlled size distribution (≤ 200 nm), suitable zeta potential values, and a good ASO encapsulation efficiency (> 60%). Additionally, these NPs show strong mucoadhesive properties in vitro, as demonstrated by Quartz Crystal Microbalance with Dissipation monitoring (QCM-D) measurements, and excellent biocompatibility with human nasal epithelial and neuronal cells. Cellular uptake *in vitro* studies show NPs internalization, while preliminary *in vivo* assessments show that intranasal administration is well tolerated, with no signs of acute toxicity in mice.
In conclusion, these nanoparticle formulations aim to enhance ASO transport across the nasal mucosa and facilitate brain uptake while ensuring safety and biocompatibility. Our findings highlight the potential of NP-mediated ASO delivery as a non-invasive alternative for brain-targeted therapies in Angelman syndrome.

References

[1] M. Gagliardi, S. Chiarugi, C. De Cesari, G. Di Gregorio, A. Diodati, L. Baroncelli, M. Cecchini, and I. Tonazzini. *Crosslinked Chitosan Nanoparticles with Muco-Adhesive Potential for Intranasal Delivery Applications.* Int. J. Mol. Sci. 24, 6590 (2023).
[2] M. Gagliardi, A. Vincenzi, L. Baroncelli, and M. Cecchini. *Stabilized Reversed Polymeric Micelles as Nanovector for Hydrophilic Compounds.* Polymers 15, 946 (2023).

Project

Angelman Syndrome Alliance (ASA) - research grant 2021 (InnovAS).

[P1.07] Neuronal extracellular vesicles as nanotools to study and monitor neurodevelopmental disorders

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Small extracellular vesicles are cell-derived nanovectors delimited by a lipid bilayer, that encapsulate a diverse cargo of proteins, lipids, and nucleic acids. These vesicles, secreted by virtually all cell types in all biological fluids, play crucial roles in various biological processes, and their molecular cargo provides valuable information about the metabolic and functional status of the parent cell [1]. Importantly, the vesicles released from neuronal cells can cross the blood-brain barrier, making them a promising source of biomarkers for the central nervous system [2]: they are a powerful tool for investigating and monitoring the CNS in both physiological and pathological conditions. Despite their potential, neuronal-derived extracellular vesicles (**NEVs**) in neuropathological models remain poorly exploited, particularly in the context of neurodevelopmental disorders.

Angelman Syndrome (**AS**) is a neurodevelopmental disorder caused by the loss of the UBE3A gene, which encodes for the ubiquitin ligase E3A (**UBE3A**) in neurons. UBE3A plays a key role in neurodevelopment but still little is known about its role in the brain. Today a therapy for AS, based on the reinstatement of UBE3A expression via antisense oligonucleotides is in clinical trial but there remains a critical need for reliable, quantitative biomarkers to assess disorder severity and track treatment efficacy beyond clinical rating scales.

We developed a clinical assay to isolate NEVs from biological fluids and use them for identifying defective biomarkers in AS murine and human models. The proteomic analysis of the NEVs' cargo showed a significant difference in the levels of several proteins between WT and AS models: these proteins are mainly involved in cell-cell adhesion, cell-matrix adhesion, cytoskeleton processes and neuronal polarization. Interestingly, UBE3A is present in WT NEVs suggesting its possible use as a direct biomarker. These results strengthened our previous observation on AS neurons that highlighted a deficit in topographical contact guidance in cells cultured on nanostructured gratings. This behavior was linked to dysregulated cytoskeleton polarization and focal adhesions' organization, with an aberrant axonal branching.

Given that this approach offers a potential window into the pathological processes of the brain: 1) the biomarkers found provide insights into novel therapeutic targets and will be instrumental for the longitudinal monitoring of AS patients, enabling the assessment of current and future therapeutic interventions while minimizing the need for more invasive procedures. Additionally, 2) this assay could be easily applicable in other neuropathological models.

References

[1] Y. Yuana, A. Sturk, and R. Nieuwland. *Extracellular vesicles in physiological and pathological conditions.* Blood Rev. 27, 31–39 (2013).[2] H. M. Ramos-Zaldívar, I. Polakovicova, E. Salas-Huenuleo, A. H. Corvalán, M. J. Kogan, C. P. Yefi, and M. E. Andia. *Extracellular vesicles through the blood–brain barrier: a review.* Fluids Barriers CNS 19, 1–15 (2022).

[P1.08] Micro patterned substrates to study peripheral nervous system pathological models

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In spite of the growing interest in the peripheral nervous system' (PNS) neurons, their role in patho-physiological conditions is still not clear. The reason is the difficulty to study sensory neurons *in vivo*, due to their sparse distribution in the skin, and the loss of their original polarization once extracted. Mechanotransduction is the conversion of external physical stimuli in biochemical signals inducing cell responses able to modify their morphology, contractility, migration or even gene expression. At cellular level, it is explicated by clusters of proteins (focal adhesions), cytoskeleton, plasma membrane and ion channels.

Piezo 2 mechanosensitive ion channels play a key role in the detection of mechanical forces in PNS, and they are predominantly expressed in dorsal root ganglia (DRG) neurons. Although Piezo 2 structure and function mechanism have been described, there is still a lack of information about its exact intracellular localization and role in processing of mechanical stimuli.

The topography surface of biomaterials is able to influence the morphological and functional properties of cells *in vitro*. We demonstrated that surface nano/micro-topographies modulate glial/neuronal differentiation, polarity, migration and neurite orientation via mechanotransduction processes [1]. Mechanical features play pivotal roles in determining cell fate too: the external stiffness can regulate PNS development and regeneration, by triggering neurite growth and the gating of Piezo channels.

Here, we have developed micropatterned substrates with alternating lines of ridges and grooves (gratings; GRs), to allow the characteristic polarized growth of peripheral neurons in a soft environment and to stimulate them with physico-mechanical stimuli. GRs, made in polydimethylsiloxane (PDMS) by solvent casting with line width of 1-10 µm, have been exploited to induce cell and neurite polarization. We investigated Piezo 2 expression and localization in HEK and DRG cells cultured on GRs, by the transfection of a Piezo 2 green fluorescent chimera.

Although PNS mechanosensory responses contribute to the arising of neurodevelopmental disorders, little is known about these processes in pathological conditions. In this framework, Ubiquitin protein ligase 3A (UBE3A) has a relevant role in neurodevelopment as changes in its expression lead to Angelman Syndrome or autism spectrum disorders [2]. Therefore, we investigated in parallel the DRG' morpho-functional responses and Piezo 2 channels in Ube3a knock-out cells cultured on our GRs.

In conclusion, GR substrates can be exploited as platforms to study in vitro the behaviour of neurons, at the mechano-sensory molecular level, as in a biomimetic environment.

References

[1] I. Tonazzini, C. Masciullo, E. Savi, A. Sonato, F. Romanato, and M. Cecchini. *Neuronal contact guidance and YAP signaling on ultra-small nanogratings*. Sci Rep. 10(1) (2020).

[2] I. Tonazzini, G. M. Van Woerden, C. Masciullo, E. J. Mientjes, Y. Elgersma, and M. Cecchini. *The role of ubiquitin ligase E3A in polarized contact guidance and rescue strategies in UBE3A-deficient hippocampal neurons.* Mol Autism. 10(1) (2019).

Project

PRIN 2020 - ToaC and PRIN 2022 (PE11)- ENGInerve.

[P1.09] β-Sheets Orientation in Physisorbed Monolayers of Proteins

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Physisorption of antibodies onto surfaces is a low-cost, rapid, and effective approach for immobilizing bioreceptors in applications such as bioelectronic sensors. [1-3] However, there is a prevailing notion that physisorbed protein layers lack structural order, thus potentially compromising their stability and sensitivity compared to antibody films that are covalently attached to the substrate surface.

We demonstrate the preferential orientation of β-sheets within the secondary structure of protein layers—specifically, anti-immunoglobulin G (anti-IgG) and bovine serum albumin (BSA) when physisorbed onto gold (Au) thin films. Using polarization modulation infrared reflection absorption spectroscopy (PM-IRRAS) and infrared attenuated total reflection (IR-ATR) spectroscopy, we provide a detailed comparative analysis of experimental PM-IRRAS data with simulated IRRAS spectra, the latter derived from optical parameters obtained via ATR data. Our findings present compelling evidence that the organization of proteins on the substrate is non-random, with notable order in their secondary structures. [4]

The similar β-sheet orientations observed in both anti-IgG and BSA films, despite their distinct secondary and tertiary structures, highlight the significant role of β-sheets in governing the structural organization of the protein films. This arrangement not only supports the stability of the films but may also enhance their functional properties, positioning physisorbed films as viable for applications where precise molecular orientation is essential. [5] These insights into molecular arrangement offer a foundation for optimizing surface interactions, thus advancing the design of biointerfaces with potential for various biomedical and biotechnological applications.

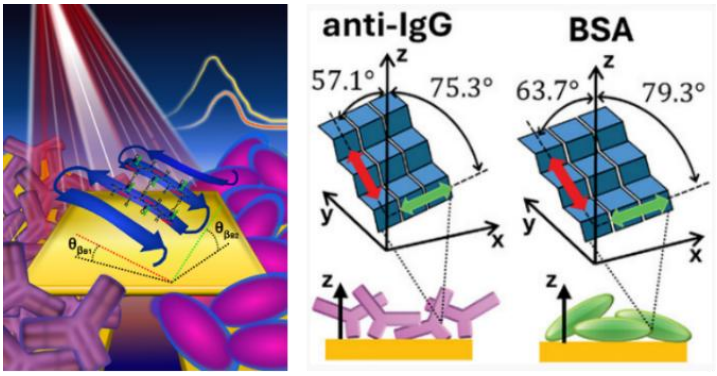

Fig. 1: The β-sheets in physisorbed layers of anti-immunoglobulin G and bovine serum albumin on gold exhibit a non-isotropic orientation, with a partial ordering that favors a tilt toward the gold surface.

References

[1] E. Macchia, et al. Advanced Materials 37, 2418610 (2025).
[2] C. Scandurra, et al. Advanced Science 11, 2308141 (2024).
[3] E. Macchia, et al. https://onlinelibrary.wiley.com/doi/abs/10.1002/adma.202309705 Advanced Materials 36, 2309705 (2024).
[4] M. Piscitelli, et al. Advanced Materials Interfaces 12, 2400867 (2025).
[5] C. Di Franco, et al. Advanced Science 12, 2412347 (2024).

[P1.10] Tunable volume plasmon polariton modes in hyperbolic metamaterials based on III-V semiconductors

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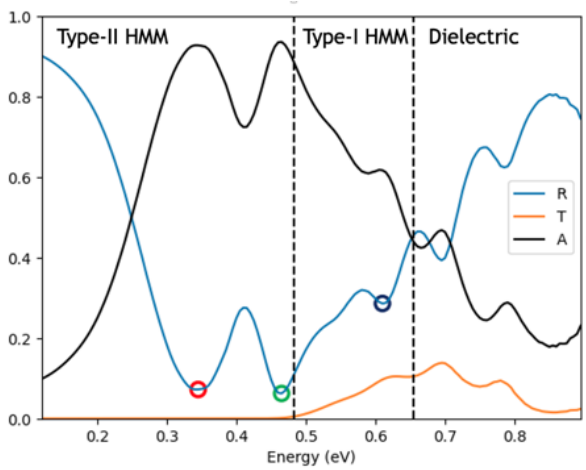
Hyperbolic metamaterials (HMMs) have gained particular attention because they allow for the propagation of electromagnetic waves with arbitrarily large wavevectors, which would be evanescent in ordinary materials. These high-k modes, called volume plasmon-polaritons (VPPs), enable advanced applications such as superlenses, sub-wavelength imaging and super-Planckian thermal emission. HMMs are characterized by extreme optical anisotropy, as they behave as metals in one direction and as dielectrics in the perpendicular direction. They are most often realized by alternating layers of metallic and dielectric systems, where plasmonic resonances are used to couple light with the metallic component of the stack. When regular metals are employed, the resulting metamaterials are generally hyperbolically active in the visible-UV range, because of their high electron density. However, HMMs working in the IR-to-THz electromagnetic range would be of great technological interest for applications in infrared optoelectronics. Recent experimental reports [1] have shown the feasibility of fabricating multilayer HMMs working in the infrared spectrum using some III-V semiconductors, where intrinsic and doped compounds serve as dielectric and metallic layers respectively.

In this work [2], we undertake a comprehensive investigation of volume plasmon polaritons within hyperbolic metamaterials. Initially, we integrate ab initio atomistic simulations based on DFT+U and the effective medium approximation to theoretically demonstrate the capability of realizing hyperbolic metamaterials using only III-V semiconductors. The obtained results are in excellent agreement with the experimental findings. However, this approach provides insights only into the first-order VPPs, so we expand beyond the limitations of effective medium theory by employing the scattering matrix method for electrodynamics simulations. This allows us to explore volume plasmon polaritons of higher orders and to predict not only the resonance peaks of transmission and reflectivity but also the electromagnetic field within the metamaterial. Moreover, by leveraging the study of the photonic band structure of the metamaterial, we systematically identify optimal excitation conditions for these resonances, independently of external environmental factors.



Several parameters can be tuned to control the excitation and the spectral characteristics of the high-k resonance modes. For instance, changing the semiconductor doping and/or the filling factor, or incorporating nanoscale structures like quantum wells can all influence the energy and the localization of Volume Plasmon Polaritons. This approach enables an efficient design of hyperbolic metamaterials, allowing one to effectively tune and harness these plasmonic resonances.

Fig. 1: Reflectivity and transmittance spectrum for the multilayer metamaterial Si:InAs/AlSb with marked volume plasmon polaritons

References

[1] P. Sohr, D. Wei, Z. Wang, and S. Law. NanoLett. 21, 9951 (2021).

[2] S. Campanaro, L. Bursi, S. Curtarolo, A. Calzolari. Submitted (2025)

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[P1.11] 3D printed devices with electro- and photoresponsive properties

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Materials with tunable shapes and properties that can be adjusted in response to external fields and environmental stimuli are crucial for a wide range of applications, including biomedicine, soft robotics, and sensing. These capabilities can be further enhanced through 3D printing technologies, which enable the creation of complex three-dimensional (3D) structures using nanostructured building blocks [1,2]. In this work, we will summarize the recent advancements from our group in developing 3D printed components whose properties can be modulated by electrical and optical fields. Specifically, we utilize ultraviolet digital light processing (DLP) to fabricate 3D components from shape memory polymers doped with carbon nanomaterials, as well as photocurable polymers doped with photoresponsive molecules. Current applications under investigation include optical processors, optical switches, and soft actuators.

References

[1] A. Camposeo, L. Persano, M. Farsari, and D. Pisignano. *Additive Manufacturing: Applications and Directions in Photonics and Optoelectronics*. Adv. Optical Mater. 7, 1800419 (2019).
[2] F. D'Elia, F. Pisani, A. Tredicucci, D. Pisignano, and A. Camposeo. *Cryptographic Strain-Dependent Light Pattern Generators*. Adv. Mater. Technol. 7, 2101129 (2022).

Project

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[P1.12] Heat Management through Bipolar Thermoelectricity in Superconducting Tunnel Junctions

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Effective heat management at cryogenic temperatures is crucial for the advancement of superconducting quantum technologies. In this study [1], we investigate the controlled manipulation of heat transfer and thermal rectification using an asymmetric superconducting tunnel junction.

Our device exhibits pronounced non-reciprocal thermal properties, generating a thermoelectric response only when heat is applied to the electrode with the larger superconducting gap [2,3]. This asymmetry significantly enhances thermal rectification, effectively enabling the device to function as an efficient heat diode.

Moreover, when operating in the thermoelectric regime, the same device acts as a heat pipe, efficiently removing excess heat from the cryogenic environment and minimizing thermal losses. Notably, this dual functionality is entirely passive, with its performance parameters easily tunable through adjustments to an external electrical load.

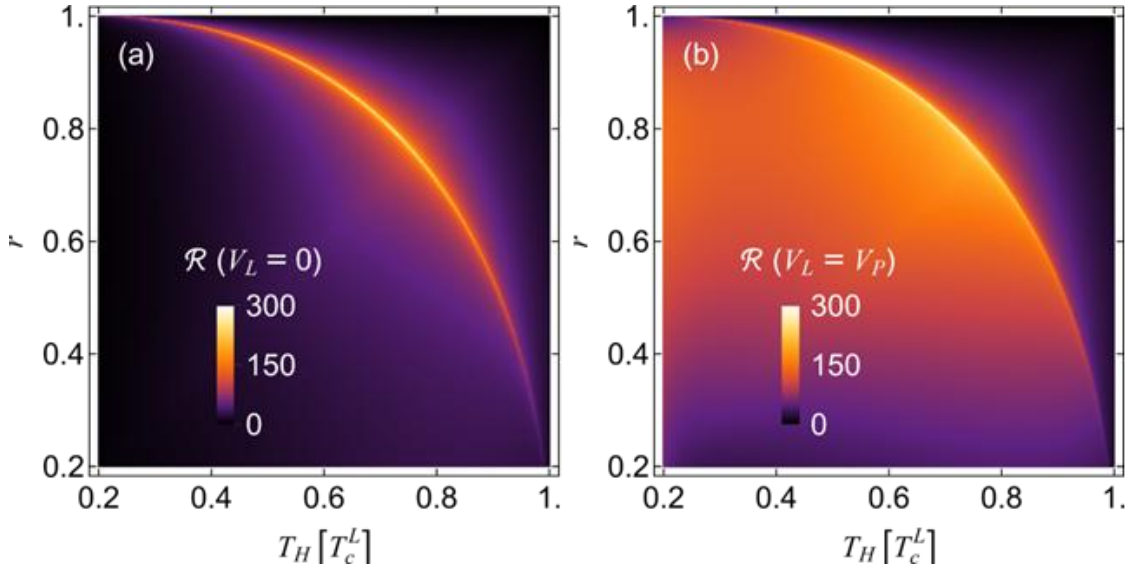

Fig. 1: Rectification efficiency R$\mathcal{R}$ as a function of the hot electrode temperature THT_H and the gap ratio rr, evaluated at an applied voltage VL=0$V_L=0$ in (a) and at the matching peak voltage VL=VP$V_L=V_P$ in (b). The matching peak VPV_P arises due to the asymmetric superconducting energy gaps, where the ratio r between the two deviates from unity.

References

[1] F. Antola, A. Braggio, G. De Simoni, and F. Giazotto. *Tunable thermoelectric superconducting heat pipe and diode.* Supercond. Sci. Technol. 37, 115023 (2024).

[2] G. Germanese, F. Paolucci, G. Marchegiani, A. Braggio, and F. Giazotto. *Bipolar thermoelectric Josephson engine*. Nat. Nanotechnol. 17, 1084–1090 (2022).

[3] G. Marchegiani, A. Braggio, and F. Giazotto. *Nonlinear Thermoelectricity with Electron-Hole Symmetric Systems.* Phys. Rev. Lett. 124, 106801 (2020).

[P1.13] InAs on Insulator as an ideal candidate for caloritronics

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In this work, we are proposing, as an ideal candidate for caloritronic devices operating at subKelvin temperatures, a hybrid superconductor-semiconductor platform named InAs on insulator (InAsOI). This heterostructure is made by doped InAs grown on an insulating buffer of InAlAs on a GaAs substrate. Caloritronic devices aim to heat or cool electrons out of equilibrium with respect to the phonon degree of freedom. However, their performances are usually limited by the strength of the electron-phonon (e-ph) coupling and the associated power loss. Our work discusses the advantages of the InAsOI platform, which are based on the significantly low e-ph coupling measured compared to all-metallic state-of-the-art caloritronic devices and the possibility of being gated. Our structure demonstrates values of the e-ph coupling constant up to two orders of magnitude smaller than typical values in metallic structures. Moreover, the possibility to manipulate the electron density (and all the connected properties) with an external electric field makes this kind of platform very appealing.

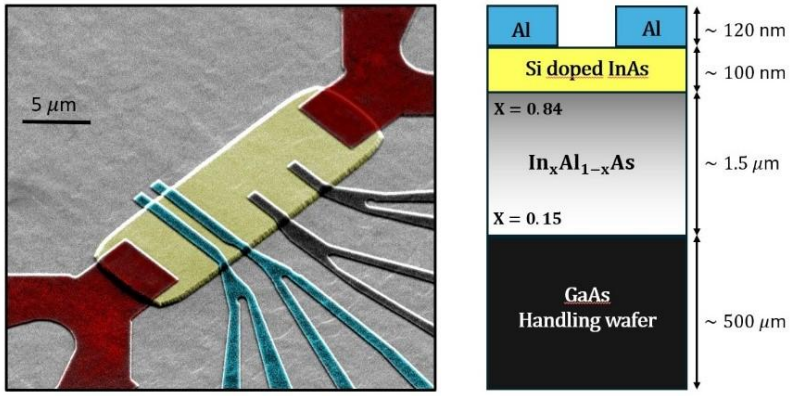

Fig. 1: On the left, a SEM (scanning electron microscopy) image of the device used for the measurements. On the right, a sketch of the InAsOI heterostructure.

[P1.14] Perfect Absorption of Single-Photons in Molecular Spin-based Quantum Circuits

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We have recently shown that it is possible to encode spin qubits into hybrid architectures obtained by integrating molecular spins into planar microwave superconducting resonators [1,2] and to use them as memories for information [1]. These hybrid architectures can work also for quantum sensing of magnetic fields, where the amplitude or the phase of an AC field synchronized with the microwave sequence driving the spin echo can be inferred [3]. Here sensitivity up to nT/Hz$---\sqrt{}nT/Hz$ can be achieved using Dynamical Decoupling [3]. However, these methods are typically limited by the spin coherence lifetime, making highly desirable the search for alternative sensing schemes.

Here we consider an open quantum system formed by molecular spin qubits strongly coupled to a lumped element superconducting Niobium resonator at mK temperature and in the single photon regime (Fig. 1) [4]. We experimentally show that it is possible to obtain points of Perfect Absorption in which zero reflectivity is observed detuned from resonance, at two symmetric positions with respect to it. Our analysis reveals that this is achieved thanks to the interplay and balance between radiative and non-radiative losses mediated by the spin detuning, which controls the spin-photon mixing of each polariton. We then show that Perfect Absorption can be observed also in the weak spin-photon coupling regime [4]. Our results largely extend the possibility to study Perfect Absorption and to exploit it in quantum technologies, with potential benefits in single-photon switches or for quantum sensing [4].

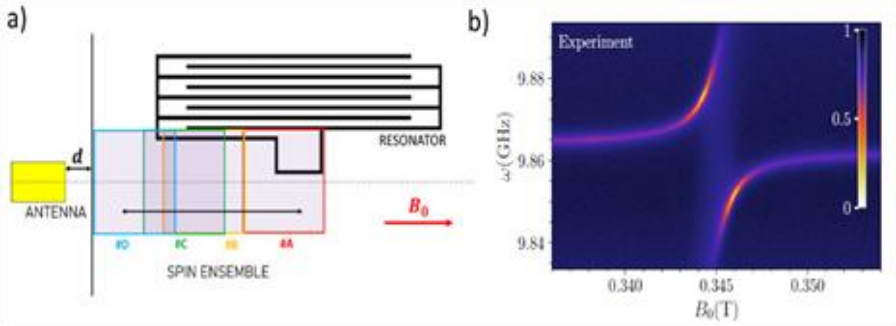

Fig. 1: a) Sketch of the microwave resonator coupled to its feeding antenna and with four sample positions (#A to #D) used in experiments. b) Reflection map showing the polaritons and the dips at which Perfect Absorption Occurs.

References

[1] C. Bonizzoni, A. Ghirri, F. Santanni, M. Atzori, L. Sorace, R. Sessoli, and M. Affronte. *Storage and retrieval of microwave pulses with molecular spin ensembles.* npj Quantum Inf. 6, 68 (2020).

[2] C. Bonizzoni, M. Maksutoglu, A. Ghirri, J. Van Tol, B. Rameev, and M. Affronte. *Coupling Sub-nanoliter BDPA Organic Radical Spin Ensembles with YBCO Inverse Anapole Resonators.* Appl. Magn. Reson. 54, 143 (2023).

[3] C. Bonizzoni, A. Ghirri, F. Santanni, and M. Affronte. *Quantum sensing of magnetic fields with molecular spins.* npj Quantum Inf. 10, 41 (2024).

[4] C. Bonizzoni, D. Lamberto, S. Napoli, S. Gunzler, D. Rieger, F. Santanni, A. Ghirri, W. Wernsdorfer, S. Savasta, and M. Affronte. *Observation of Perfect Absorption in Hyperfine Levels of Molecular Spins with Hermitian Subspaces.* In preparation (2025).

[P1.15] Biharmonic-drive tunable Josephson diode

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The superconducting diode effect has gained significant attention for its potential applications in cryogenic electronics and quantum computing, offering zero resistance and no energy loss in the forward direction [1]. The effect was demonstrated in various superconducting platforms including spin-orbit-based Josephson junction, van der Waals materials and interferometric devices. These devices often require peculiar materials with broken spatial symmetries or the application of magnetic field to break time reversal, making them challenging to scale and integrate into computer chips and quantum devices. Here, we present a novel approach to achieve the superconducting diode effect by breaking spatio-temporal symmetries in an Al-InAs-based Josephson junction using a biharmonic AC drive signal [2]. Using an antenna, we obtain wireless control of the diode polarity and efficiency, making it scalable and adaptable. Our experimental results show a tunable diode efficiency up to the ideal 100% over a wide frequency range, signal rectification and temperature resilience up to 800 mK. This highly adaptable, platform-independent diode represents a promising building block for future superconducting digital electronics, including efficient logic gates and ultra-fast switches.

References

[1] M. Nadeem, M. S. Fuhrer, and X. Wang. *The superconducting diode effect.* Nat Rev Phys 5, 558–577 (2023).
[2] D. Scheer, R. S. Souto, F. Hassler, and J. Danon. *Tunable diode effect in a superconducting tunnel junction with biharmonic drive.* New Journal of Physics 27 (2025).

[P1.16] Proposal of interferometric sensing of gate-induced microscopic effects in superconducting quantum devices

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Radio-frequency reflectometry was introduced in 1998 as a high-sensitivity, high-bandwidth measurement technique for single-electron devices [1]. Here, we propose an alternative method for measuring extreme impedances known as active interferometry [2]. In this approach, the wave reflected off the device is canceled out with another wave of the same frequency and magnitude, but with a 180° phase offset. Selecting any measurement frequency is a significant advantage of active interferometry over other high-sensitivity solutions based on resonators, which inevitably constraint the probing frequency. We suggest to apply this technique to detect possible single-particle poisoning events in superconducting weak links activated by nearby gate electrodes. This research could enhance the understanding of the gate-controlled supercurrent mechanism [3].

References

[1] R. J. Schoelkopf et al. *The radio-frequency single electron transistor (RF-SET): a fast and ultrasensitive Electrometer*. Science 280, 1238-42 (1998).

[2] G. Vlachogiannakis, et al. *An I/Q-mixer-steering interferometric technique for high-sensitivity measurement of extreme impedances*. IEEE MTT-S International Microwave Symposium, IMS 2015, May 17, 2015 - May 22, 2015, Phoenix, AZ, United States (2015).

[3] G. De Simoni, et al. *Metallic supercurrent field-effect transistor*. Nat. Nanotech. 13, 802 (2018).

[P1.17] Exploiting the interaction of Abrikosov vortex pattern and supercurrent crowding to control supercurrent rectification

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Diodes, including pn and Schottky junctions, are components that allow current to flow in a single direction due to their broken spatial symmetry. These widely used semiconductor devices serve various roles, from photon detection and emission to signal rectification. Similarly, superconducting electronics, thanks to its high energy efficiency and elevated operating frequencies, has seen substantial advancements, with numerous superconducting counterparts to conventional semiconductor devices being now available. Supercurrent diodes (SDs) are among these innovations. They leverage non-reciprocal lossless Cooper pair transport to exhibit distinct forward and reverse switching currents [1]. Despite considerable research, a definitive platform for SD realization has yet to emerge. In this work, we present a superconducting diode based on asymmetric Dayem Bridge Josephson junctions, where the supercurrent crowding [2] and Abrikosov vortex pinning [3] are utilized to tailor and regulate the superconducting diode phenomenon. Experimental prototypes built on this concept are introduced, supported by time-dependent Ginzburg-Landau modeling to elucidate the observed behavior.

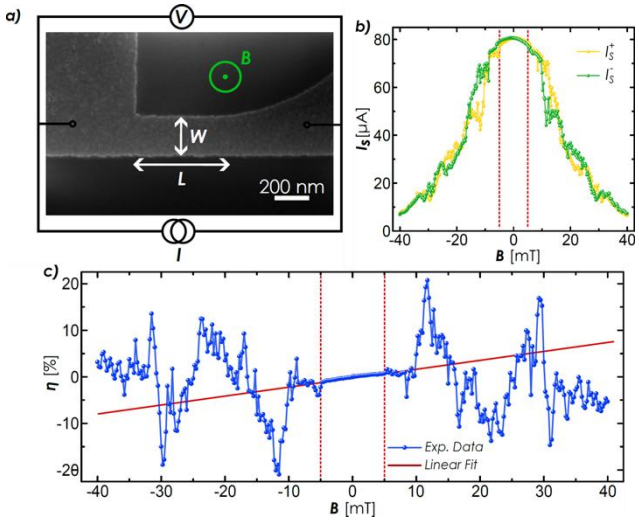

Fig. 1: a) SEM image of an asymmetric Dayem Bridge supercurrent diode and schematic of the measurement setup. b) Positive and negative switching current values I_s^+ and I_s^+ vs. the out of plane external magnetic field B of a representative device. The red dashed lines indicate the regime dominated by Meissner currents. c) Evolution of the rectification parameter η. The dashed lines have the same meaning as in panel b, while the red solid line represents the linear fit to the data in this regime.

References

[1] F. F. Ando, et al. *Observation of superconducting diode effect*. Nature 584, 373–376 (2020).

[2] O. A. O. A. Adami, et al. *Current crowding effects in superconducting corner-shaped Al microstrips*. Appl. Phys. Lett. 102, 052603 (2013).

[3] M. Foltyn, et al. *Probing Confined Vortices with a Superconducting Nanobridge*. Phys. Rev. Applied 19 (2023).

[P1.18] Coherent microwave comb generation via the Josephson effect

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We present a novel device for generating frequency combs in the microwave regime based on a superconducting quantum interference device (SQUID) driven by a time-dependent magnetic flux. The flux drive induces sharp periodic voltage spikes across the SQUID, which in the frequency domain correspond to an evenly spaced comb centered in 0 Hz.

The emitted frequency comb extends for several GHz, showing about a hundred of harmonics. It is fully tunable in amplitude and inter-teeth spacing by adjusting the flux modulation frequency, amplitude and offset.

The produced radiation exhibits long coherence times, extending up to several seconds for the single mode. We also show a well-defined constant phase relation among the comb teeth.

Experimental results demonstrate excellent agreement with numerical simulations performed using SPICE-based circuit models.

Having a small footprint (<100 um), our approach provides a compact solution for generating coherent microwave tones in cryogenic environments, addressing frequency crowding issues in superconducting circuit architectures. The demonstrated device has potential applications in cryogenic microwave electronics, quantum computing, and metrology, paving the way for new techniques in frequency synthesis and signal processing in low-temperature environments.

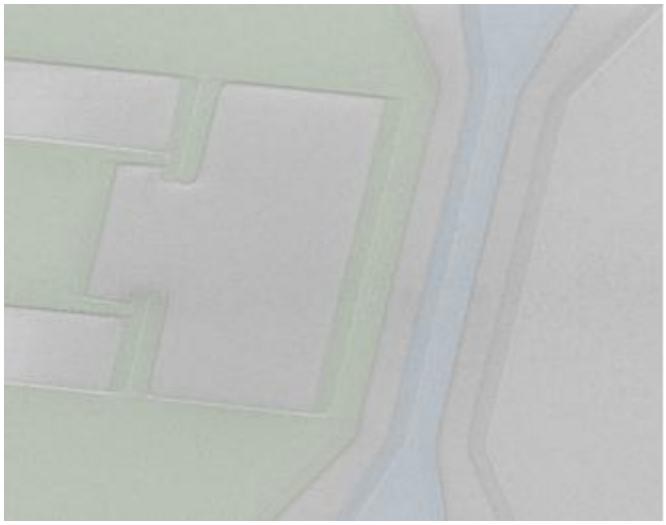

Fig. 1: SEM micrograph of the frequency comb generator.

[P1.19] Superconducting Quantum Interference Devices based on InSb Nanoflag Josephson Junctions

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In mesoscopic physics, interference effects play a major role in determining the behavior and the transport properties of quantum devices. Superconducting quantum interference devices, known as SQUIDs, are particularly important in applications regarding quantum computing, magnetometry, scanning probe microscopies, and others. Besides, SQUIDs are also used to directly measure fundamental properties of Josephson junctions, like the Current Phase Relationship (CPR).
Here we report the fabrication and characterization of SQUIDs made with InSb nanoflag-based Josephson junctions [1]. These devices are the first DC-SQUIDs realized with two-dimensional nanostructures of InSb [2]. Making use of the elongated shape of the nanoflags, both symmetric and asymmetric SQUID geometries are realized. Characterization at low temperature is performed by magneto-transport measurements, showing supercurrent interference for various values of temperature and back gate.
In the symmetric geometry, the typical SQUID interference pattern is observed. Interference can be controlled by the back gate, which allows to tune from partial to total destructive interference. An additional tuning knob is the applied perpendicular magnetic field, which allows us to choose a working point within the single junction "Fraunhofer" pattern.
In the asymmetric geometry, the different response of the two nanoflags to the global back gate leads to the disappearance of interference for certain working points, as shown in Figure 1. In the asymmetric geometry, the different response of the two nanoflags to the global back gate leads to the disappearance of interference for certain working points, as shown in Fig. 1. SQUID-type oscillations are present at back gate voltage V_{bg} = 4.5 V or higher, but not at V_{bg} = 4.0 V, where the supercurrent in one Josephson junction has been suppressed.

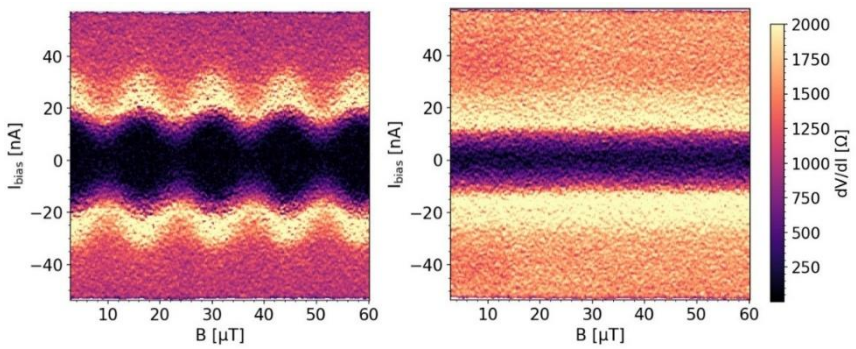

Fig. 1: Interference pattern of an asymmetric SQUID. Left: at V_{bg} = 4.5 V. Right: at V_{bg} = 4.0 V.

References

[1] S. Salimian, M. Carrega, I. Verma, V. Zannier, M. P. Nowak, F. Beltram, L. Sorba, and S. Heun. *Gate-controlled supercurrent in ballistic InSb nanoflag Josephson junctions.* Appl. Phys. Lett. 119, 214004 (2021).

[2] I. Verma, S. Salimian, V. Zannier, S. Heun, F. Rossi, D. Ercolani, F. Beltram, and L. Sorba. *High-mobility free-standing InSb nanoflags grown on InP nanowire stems for quantum devices.* ACS Appl. Nano Mater. 4, 5825 – 5833 (2021)

[P1.20] Quantum THz frequency Light: perspectives and future of next generation of Terahertz metrological sources

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The development of miniaturized terahertz (THz) quantum cascade laser (QCL) frequency combs (FCs) has rapidly impacted the field of quantum optics, condensed matter physics, and precision metrology [1]. QCL FCs exploits huge Kerr optical non-linearities and spatial hole burning effects that infer them an inherently high quantum coherence, potential for the generation of squeezed states, continuous variable entangled states, and for devising on-chip integrated compact quantum platforms [1]. Advancements in the nanofabrication of sophisticated cavity architectures and materials engineering, recently provided an unprecedented exceptional control over the emission characteristics of this class of sources, including frequency tunability, short pulse emission, and spectral purity [2, 3, 4]. The design flexibility recently allowed the integration of low-dimensional quantum materials [5], opening new pathways for achieving nonclassical THz emission regimes.

This work outlines the principles, design strategies, and potential architectures for scalable THz quantum emitters, while also addressing key challenges related to integration, thermal management, and quantum noise. The miniaturization of these sources paves the way for portable, robust, and high-precision THz metrological tools, opening new and exciting frontiers in both applied and fundamental science.

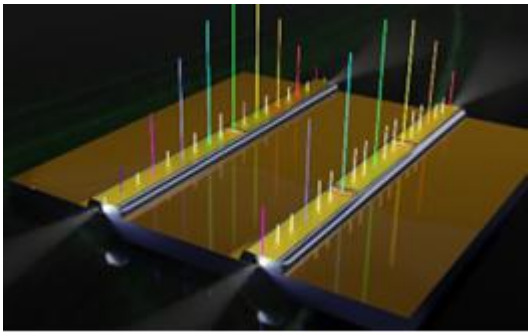

Fig 1: Engineered Fabry-Perot THz harmonic frequency comb with graphene scatters on the metallic top contact, allowing for steady comb emission at a specific harmonic order.

References

[1] M. S. Vitiello and P. De Natale. *Terahertz Quantum Cascade Lasers as Enabling Quantum Technology.* Adv Quantum Technol 5, 2100082 (2022).

[2] E. Riccardi, et al. *Short pulse generation from a graphene-coupled passively mode-locked terahertz laser.* Nature Photonics 17, 607–614 (2023).

[3] L. Consolino, et al. *Quantum cascade laser-based hybrid dual comb spectrometer.* Communication Physics 3, 69 (2020).

[3] M. S. Vitiello, et al. *Quantum-limited frequency fluctuations in a terahertz laser.* Nature Photonics 6, 525–528 (2012).

[4] E. Riccardi, M. A. Justo Guerrero, et al. *Sculpting harmonic comb states in terahertz quantum cascade lasers by controlled engineering.* Optica 11, 412-419 (2024).

[5] M. A. Justo Guerrero, et al. *Harmonic quantum cascade laser terahertz frequency combs enabled by multilayer graphene top-cavity scatters.* Nanophotonics 13, 1835–1841 (2024)

[4] E. Riccardi, M. A. Justo Guerrero, et al. *Sculpting harmonic comb states in terahertz quantum cascade lasers by controlled engineering.* Optica 11, 412-419 (2024).

[5] M. A. Justo Guerrero, et al. *Harmonic quantum cascade laser terahertz frequency combs enabled by multilayer graphene top-cavity scatters.* Nanophotonics 13, 1835–1841 (2024).

[P1.21] Probing spin-electric transitions in a molecular exchange qubit

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Electric fields represent an ideal means for controlling spins at the nanoscale and, more specifically, for manipulating protected degrees of freedom in multispin systems. Here we perform low-temperature magnetic far-IR spectroscopy on a molecular spin triangle (Fe3) and provide initial experimental evidence suggesting spin-electric transitions in polynuclear complexes. The co-presence of electric- and magnetic-dipole transitions, allows us to estimate the spin-electric coupling. Based on spin Hamiltonian simulations of the spectra, we identify the observed transitions and introduce the concept of a generalized exchange qubit. This applies to a wide class of molecular spin triangles and includes the scalar chirality and the partial spin sum qubits as special cases [1].

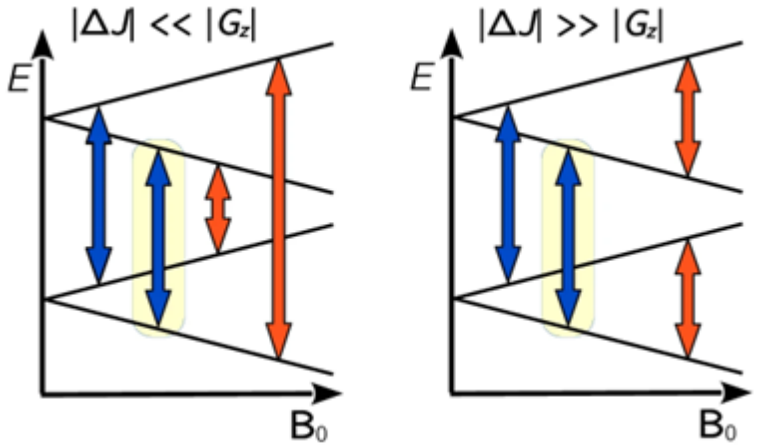

Fig. 1: Schematic representation of the electric-dipole (blue arrows) and magnetic-dipole transitions (red arrows) between the lowest states of the molecular spin triangle. The schemes refer to the limiting cases of a chirality (left) and of an exchange qubit (right), corresponding to an exchange inhomogeneity (ΔJ) that is smaller or larger than the Dzyaloshinskii–Moriya interaction (G_z), respectively.

Reference

[1] F. le Mardelé, I. Mohelský, J. Wyzula, M. Orlita, P. Turek, F. Troiani, and A. K. Boudalis. *Probing spin-electric transitions in a molecular exchange qubit.* Nature Communications 16, 1198 (2025).

[P1.22] A strategy to enhance stability and photoactivity of Cu_xO systems for water splitting

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Photocatalytic water splitting is a promising approach to produce green hydrogen. Copper oxides have attracted significant attention as photocatalysts due to their visible-range band gap, non-toxicity, earth abundance and favorable band positions for water splitting. However, semiconductor-based systems suffer from low photocatalytic efficiency due to the rapid recombination of the photogenerated electron-hole pairs. The construction of a heterojunction photocatalyst can overcome this challenge by providing spatial charge carrier separation. In this study, we investigated the photocatalytic activity of CuO and Cu_2O. Moreover, we focused on the development of a heterojunction system composed of Cu nanoparticles coated with a Cu_2O shell (Fig. 1). This architecture allows energy transfer through multiple pathways, reducing the massive loss of the electron-hole pairs. Furthermore, Cu NPs exhibit a localized surface plasmon resonance (LSPR) peak in the near-infrared region, which extends the solar absorption range of the photocatalytic system (Fig. 1). CuO and Cu_2O reference samples, as well as the $Cu@Cu_2O$ core@shell NPs, were grown using molecular beam epitaxy. The growth procedure for all samples was optimized, as the oxidation state is highly dependent on pressure, temperature, and oxygen exposure during growth [1]. The surface chemical composition of the samples was monitored via X-ray photoelectron spectroscopy, while UV-Visible absorption spectroscopy was used to study the optical properties. Transmission electron microscopy provided information about the morphology and size of the NPs. The photoelectrochemical measurements, conducted at the Physics Department of Bologna, confirmed the photodegradation of copper-based systems in aqueous environments. Hence, capping strategies were explored to enhance photostability. Additionally, ultrafast transient absorption spectroscopy studies were performed at Cnr-ISM in Rome. The photoexcitation dynamics of the samples was studied by pumping both at the plasmonic resonance and above the band gap of the oxides. The data show evidence for a charge transfer from the metallic core to the oxide shell upon photoexcitation of LSPRs.

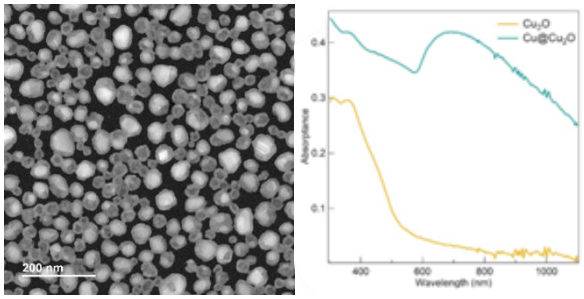

Fig. 1: STEM image of Cu@Cu2O NPs (left); absorptance spectra which highlight the extended absorption range of $Cu@Cu_2O$ compared to Cu_2O alone (right).

Reference

[1] E. Spurio, G. Bertoni, S. D'Addato, F. Alimonti, and P. Luches. *Mapping the local stoichiometry in Cu nanoparticles during controlled oxidation by STEM-EELS spectral imaging.* Nanoscale 17, 4132–4141 (2025).

[P1.23] From the orchard with LOVE: acoustic wave-based polyphenols detection to improve the olive value chain

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The olive value chain is considered part of the Italian excellence in food production and often verified with the "Made in Italy" certification. To comply with the required standards, the whole production chain heavily relies on quality assessments to guarantee product integrity and consumer health. From the ripeness of the olives now of harvest to the final characteristics of the olive derivatives (oil, paste, pickled olives, …) thorough quality checks are essential to ensure authenticity, safety, and preservation of the organoleptic properties. Olive fruits are rich in some specific polyphenols such as hydroxytyrosol, tyrosol, oleocanthal, oleacein, oleuropein, verbascoside and caffeic acid, and their overall concentration can serve as a marker for the ripeness degree [1], which is a key parameter to consider in order to minimize waste and to ensure the highest fruit quality when settling the harvest time. However, the detection of polyphenol content is still expensive and time-consuming, since it goes through analytical methods such as mass spectrometry, chemiluminescence, electroanalysis, and chromatography [2]. In contrast to the current approach involving sample collection, laboratory shipment, and result delays, the LOVE project (Lab-on-chip for sustainable Olive ValuE chain) proposes a simplified, cost-effective, and time-efficient strategy for evaluating the phenolic content in olives thanks to a Quartz Crystal Microbalance with Dissipation monitoring (QCM-D). This innovative approach relies on an acoustic sensor functionalized with an analyte-specific probe [3] that enables rapid detection of polyphenols in olive extracts. The development of a simplified procedure can pave the way to produce a portable device that could allow for on-field determination of the ripening degree of olive drupes, with the aim of improving the harvesting step in the crafting of premium olive derivatives.

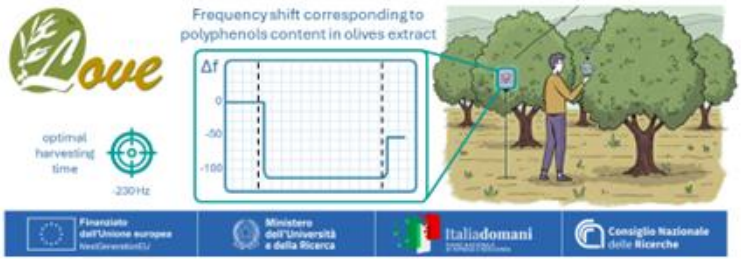

Fig. 1: project logo and working principle of the QCM-based sensor.

References

[1] G. Vicario, C. Cantini, A. Francini, A. Raffaelli, M. Cifelli, V. Domenici, and L. Sebastiani. *Olive Fruit Ripening Degree and Water Content Relationships with Phenolic Acids and Alcohols, Secoiridoids, Flavonoids and Pigments in Fruit and Oil.* Molecules 28, 6943 (2023).

[2] B. Li, J. Lecourt, and G. Bishop. *Advances in Non-Destructive Early Assessment of Fruit Ripeness towards Defining Optimal Time of Harvest and Yield Prediction—A Review.* Plants 7, 3 (2018).

[3] M. Gagliardi, G. Tori, M. Agostini, F. Lunardelli, F. Mencarelli, C. Sanmartin, and M. Cecchini. *Detection of Oenological Polyphenols via QCM-D Measurements.* Nanomaterials 12, 166 (2022).

Project

PRIN 2022 - Cod. 2022M4WB3M (LS9) LOVE – "Lab-on-chip for sustainable Olive ValuE chain" - CUP B53D23017860006, funded by the European Union – Next Generation EU in the context of the Italian National Recovery and Resilience Plan.

[P1.24] Physical synthesis and investigation of core@shell nanoparticles

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The use of physical synthesis of nanoparticles (NP) offers advantages, as it is single-step and ligand-free. These characteristics enhance the precision of NP structure analysis and elucidate their properties more accurately. In our group various types of NPs have been prepared and studied, with a gas aggregation source and with thermal evaporators. Techniques like co-deposition and sequential layer deposition have been exploited in fabricating core@shell NPs. These methodologies have enabled the creation of non-native oxide shells, easing the exploration of metal@metal oxide core@shell NPs by independently varying core diameter and shell thickness. This paper presents findings on physically synthesized Cu@CaF_2, Ag@CaF_2 and Cu@MgO NPs, which can be significant due to their potential for enhancing power cell efficiency in photovoltaic devices through Surface Plasmon Resonance (SPR) [1]. The characterization of NP assembly involved techniques such as SEM, TEM, AFM, in situ XPS and UV-VIS absorption spectroscopies. These analyses establish correlations between SPR behavior, film morphology, and core/shell interface properties, stressing the crucial role of precise synthesis procedures in tailoring the optical properties of these systems.

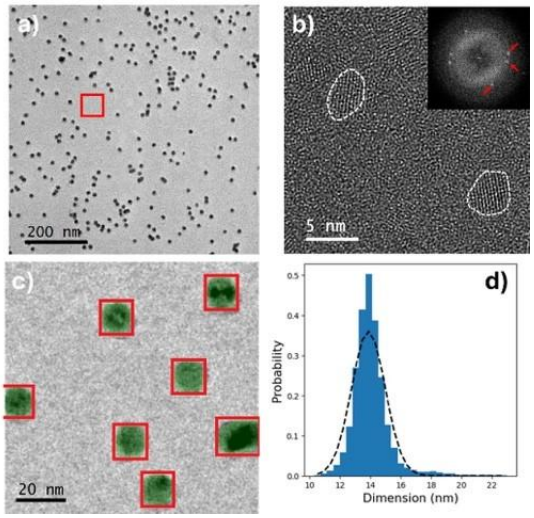

Fig. 1: a) TEM image of Cu NPs on CaF2 b) HR-TEM acquired in the red-squared region in (a): the small crystals reveal the polycrystalline nature of the CaF2 film. The inset shows the associated FFT.c) Detection and segmentation of Cu NPs using Mask R-CNN, showing bounding boxes and segmentation masks around individual particles. d) Diameter distribution of Cu NPs obtained from the statistical analysis of 30 TEM images, covering a total of 5392 particles.

Reference

[1] S. D'Addato and M. C. Spadaro. Invited Comment. Phys. Scr. 93, 033001 (2018).

Project

PNRR MUR project ECS_00000033_ECOSISTER. European Union - NextGenerationEU.

[P1.25] Electrically tunable optical properties of hybrid oxide multilayers

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TCOs, with their unique combination of optical transparency and electrical conductivity, are fundamental to photovoltaics and optoelectronics [1]. Their tunable carrier density allows for precise control of "*epsilon-near-zero*" effects, crucial for optical communication [2]. Although doping enables static property adjustment [3], external stimuli-driven control is highly desired to enable the next generation of photonic devices. Using a plane capacitor with a 500 mm SrTiO3 dielectric, we achieved AZO gating in a prior study [4], but this design demanded high voltage and cryogenic conditions for significant charge displacement.
We present the successful fabrication and detailed characterization of hybrid Al-doped ZnO/$BaTiO_3$ multilayer structures grown on Nb-doped $SrTiO_3$ substrates, demonstrating room-temperature optical modulation with remarkably low applied voltages. Through in-operando spectroscopic ellipsometry, we observed significant voltage-induced variations in the refractive index of the AZO layer, with changes exceeding 2 at an applied bias of only 3V. These variations are attributed to a synergistic combination of charge accumulation at the insulator/semiconductor interface and the field-induced Pockels effect within the $BaTiO_3$ layer, a finding that was successfully validated by an optical model incorporating these physical mechanisms. This demonstration of a substantial electro-optic response [5] confirms the suitability of these oxide heterostructures for the development of highly efficient, voltage-modulated active optical systems.

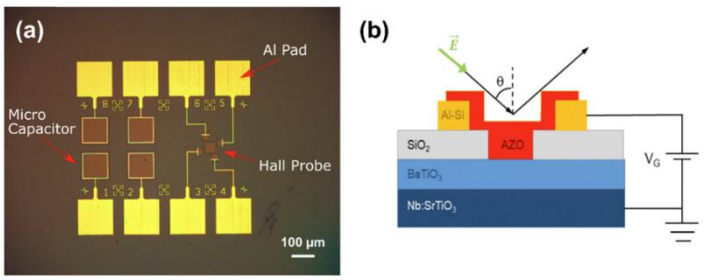

Fig. 1: (a) Microcapacitors fabricated via EBL. (b) Cross-section of the stacking of the layer films.

References

[1] T. Minami. Semicond. Sci. Technol., 20, S35–S44 (2005).
[2] K. Ellmer. Nat. Photonics, 6, 808–816 (2012).
[3] N. Kinsey, et al. Optica, 2, 616–622 (2015).
[4] X. Niu, X. Hu, S. Chu and Q. Gong. *Epsilon-Near-Zero Photonics: A New Platform for Integrated Devices.* Adv. Opt. Mater. 6, 1701292 (2018).
[5] A. K. Pradhan, et al. *Extreme tunability in aluminum doped Zinc Oxide plasmonic materials for near-infrared applications.* Sci. Rep. 4, 6415 (2014).
[6] I. Valenti, et al. Electrical*, optical, and electronic properties of Al:ZnO films in a wide doping range.* J. Appl. Phys., 2015, 118, 165304 (2015).
[7] M. Sygletou, et al. *In-Operando Optical Spectroscopy of Field-Effect-Gated Al-Doped ZnO*. ACS Appl. Mater. Interfaces 3112 (2023).
[8] R. Magrin Maffei, et al. Active J. Mater. Chem. C (2025).

[P1.26] Opto-electronic properties of amorphous ITO-ZnO mixed oxide transparent conducting films

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Amorphous transparent conducting oxides (a-TCOs) are of great interest in next-generation optoelectronic devices because they combine high optical transparency, low electrical resistivity, with higher mechanical strength, absence of grains, and ease of processing [1]. This work investigates the relationship among structural, optical, and electrical properties of ITO-ZnO mixed oxide films prepared by co-sputtering technique at room temperature. Systematic compositional tuning in the mixed oxide optimizes the structural, optical, and electrical properties [2]. The cation ratio (d) of In/(In + Zn) is varied from 0 to 0.5 in the ITO-ZnO mixed oxide, and the corresponding crystalline structure evolved from polycrystalline to an amorphous-like structure, indicating higher In content favors amorphization. However, a polycrystalline peak for the homologous compound of $Zn_xIn_3O_{3+x}$ is found for d = 0.13 (Fig. 1a). Comparatively higher Urbach energy value is also obtained for the amorphous-like films (Fig. 1b). The average visible transparency value decreased from 79.2% to 75.4%, with an increase in d value from 0 to 0.5. Similarly, the resistivity value decreased from 6.29×10^{-1} to 8.22×10^{-4} W-cm, with an increase in d value from 0.13 to 0.5, and the corresponding mobility value increased from 13.3 to 27.5 cm^2/V-s, indicating that the amorphization nature is suitable for better electrical properties. Furthermore, the optical band-gap value also increases with an increase in In content, which is at par with the electrical carrier concentration values (Fig. 1b). X-ray photoelectron spectroscopy confirms the chemical states of In, Zn, and Sn in the mixed oxide. Overall, this investigation indicates that the In content can tune the structural, optical, and electrical properties of co-sputtered ITO-ZnO mixed oxide films-based a-TCOs to achieve better transparency and conductivity films for optoelectronic and plasmonic applications.

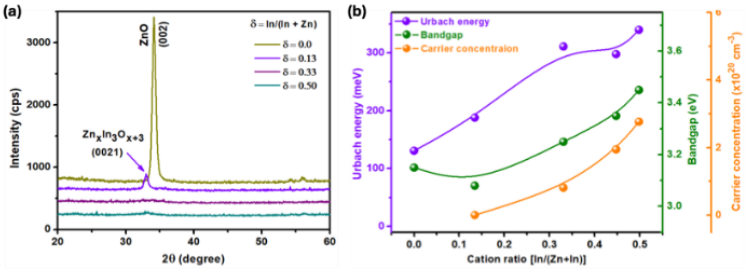

Fig. 1: (a) X-ray diffraction patterns and (b) opto-electrical properties of ITO-ZnO mixed oxides for different cation ratios.

References

[1] T. Koida and J. Nomoto. *Sustainable Transparent Conducting Oxides: Insights from Amorphous SnO_X Thin Films via Oxygen Stoichiometry Control.* Chem. Mater. 36, 6838–6848 (2024).

[2] J. Sheng, et al. *Flexible and High-Performance Amorphous Indium Zinc Oxide Thin-Film Transistor Using Low-Temperature Atomic Layer Deposition*, ACS Appl. Mater. Interfaces 8, 33821−33828 (2016).

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[P1.27] Friction induced tribovoltaic charge generation in metal - semiconductor junction

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Triboelectric nanogenerators operate on the mechanisms of contact electrification and electrostatic induction. Various material couplings have been tested and classified based on their surface charge effects [1]. The voltage output in these scenarios is alternate (AC voltages), consequently needing rectification prior to utilization. This creates the need of DC voltage sources which can be used without incurring any losses during rectification on portable or large-scale applications. In this respect, tribovoltaic nanogenerators (TVNGs) produce such DC voltage outputs on many material couplings. In a p-n junction, a TVNG operates on the mechanism of electron-hole pairs created as a result of the energy released by the creation-breaking of chemical bonds at the interface due to mechanical sliding [2]. The arising voltages are affected by contact pressure (load) and by the sliding velocity.

In this work, a reciprocating ball-on-plate module of a standard tribometer (CETR UMT-3) was implemented, so to measure in real-time the generated tribo-voltage. A dynamic conventional Schottky junction was obtained by sliding an Aluminium ball against a Silicon substrate 2 mm thick (Si-Al), as depicted in Fig. 1a. A low-friction and a high-friction region with different electrical responses is shown below. These two phases of the tests are ascribed to different wear of both the counter bodies, and the consequent production of debris. Fig. 1b shows a case study of Si-Al pair with sections marked for low-friction (CoF ≈ 0.6, Fig. 1c) and high-friction (CoF ≈ 0.9, Fig. 1d) regions. In both the regions the electric signals observed are periodic DC signals, reflecting the trend of the CoF related to the reciprocating motion. The highest voltage peaks observed in the high friction region, being about ~ 240 mV, while in the low friction region the peak is about ~ 15 mV at the applied conditions. However, in the high friction region a threshold can be identified above which the voltage increases further and spans even negative values. This unstable behaviour is ascribed to extensive wear of the surfaces and transferring of material.With the aim of giving further insights on this topic, other different materials will be coupled together.

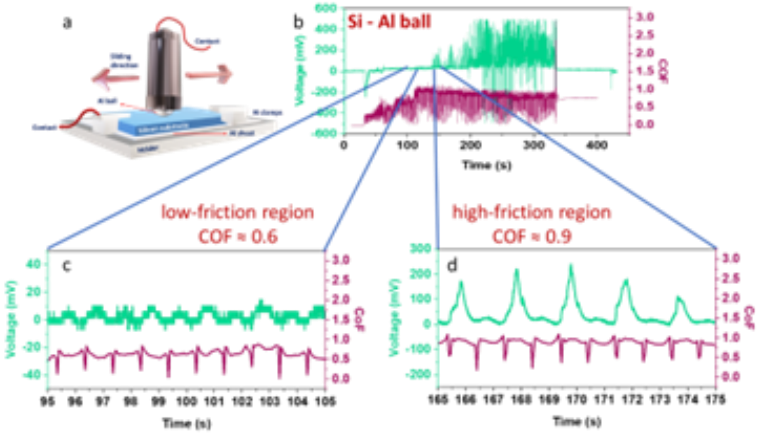

Fig. 1: (a) Representation of the triboelectric setup, (b) Case study of Si-Al pair under an applied load of 20 N and a sliding velocity of 15 mm/s, focused area for (c) low-friction and (d) high-friction regions.

References

[1] C. Wu, et al. *Triboelectric Nanogenerator: A Foundation of the Energy for the New Era.* Adv. Energy Mater. 9, 1802906 (2019).

[2] S. Lin and Z. L. Wang. *The tribovoltaic effect.* Materials Today 62, 111-128 (2023).

[P1.28] Electron microscopy toward quantum measurements

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Transmission Electron microscopy is a powerful tool to image and analyze materials and nanostructures. However, our group's research aims to extend quantum methodologies and concept to extend TEM's measurement possibilities.
I will highlight some of the directions and some results already achieved. For example, we will describe here the progress in quantum state tomography in the OAM states and how this is going to help the progress in electron microscopy and spectroscopy.
Progressing along this same line there is also the possibility to produce efficient electron light interaction for experiments of interferometry in the energy domain.
This will be a very important tool for new interferometric experiments like Ramsey holography of inelastic scattering. Future applications in quantum materials are also briefly discussed.

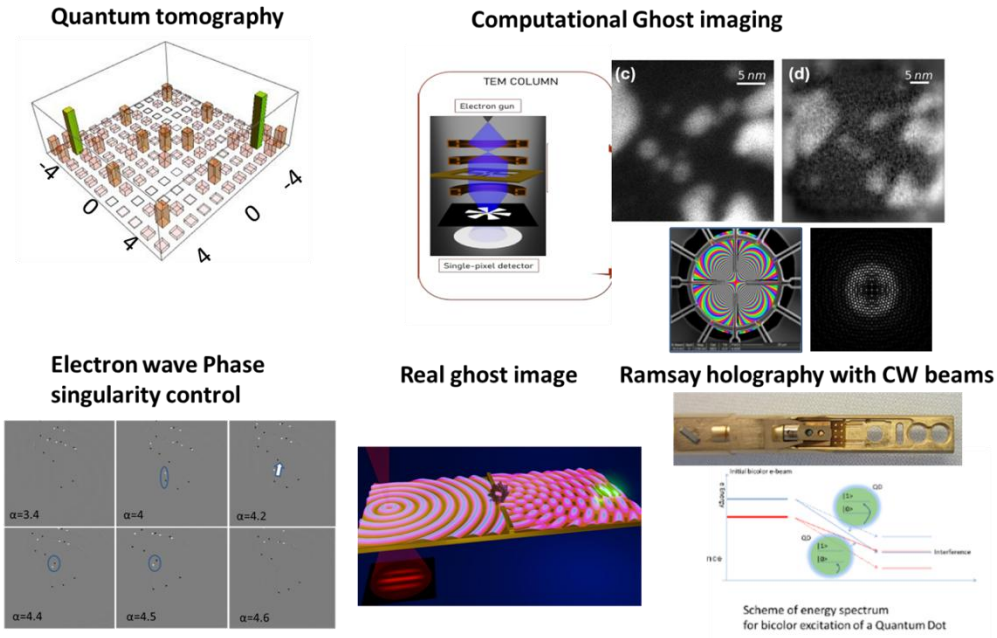

Fig. 1: Some of the directions of quantum developments in our TEM research: a) first quantum state tomography in OAM basis, b) computational ghost imaging c) Control of phase singularities and "Hilbert Hotel" experiments d) real ghost imaging using entanglement e) Ramsey holography and two state interference to measure phase in inelastic scattering.

[P1.29] Control of the Enhanced Dielectric Properties of Nanostructured Complex Oxides via Cluster-Assembling

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Colossal dielectric constant (CDC) materials, having extremely high dielectric permittivity ($\varepsilon' > 10^3$), are critical for various technological applications. If ε' is sufficiently large, it allows the development of transparent CDC devices, such as transparent capacitive batteries, which are highly required for numerous advanced applications. Among other materials, wurtzite Zinc Oxide (ZnO) has gained considerable attention due to its wide bandgap of 3.37 eV and high exciton binding energy of 60 meV, making it the best choice for CDC-based applications [1,2].

In our study, ZnO nanoparticles were synthesized via supersonic cluster beam deposition which is a gas phase technique under ultra-high vacuum. To study the tunability of their dielectric properties, time-dependent doping was done using gadolinium chloride (GdCl) and iron chloride (FeCl). The ZnO nanoparticles were soaked in prepared solutions of these dopants to enable the incorporation of Gd and Fe ions into the ZnO lattice. Annealing at 400°C was carried out to study its effects on the crystallinity and morphology of the prepared films.

X-ray photoelectron spectroscopy (XPS) was used to analyze the elemental composition and valence states of the doped ZnO films. The XPS spectra confirmed that Gd and Fe was successfully incorporated into the ZnO lattice, with characteristic peaks corresponding to Zn (Zn 2p), oxygen (O 1s), carbon (C 1s), gadolinium (Gd 3d), and iron (Fe 2p). Especially, no impurity-related peaks were detected, which is further validation of the purity and effectiveness of the adopted doping process.

Raman spectroscopy is a powerful non-destructive tool which utilizes inelastic scattering. It provides information on vibrational modes, structural orientation, crystallinity, and impurities. Raman was performed to analyze the vibrational modes of the ZnO films. However, when ZnO films are grown on silicon substrates, the Raman spectrum dominates by silicon signals, leading to a weaker ZnO Raman scattering. Despite this challenge, Raman spectroscopy successfully investigated ZnO-related vibrational modes, including the A1(LO) and E2 modes, which confirms the structural integrity of the doped ZnO films.

Characterizing extremely small nanoparticles by using conventional lab-based X-ray diffraction (XRD) is more challenging due to its limited resolution and sensitivity. Therefore, for further structural analysis of the prepared nanoparticles, synchrotron-based powder diffraction (XPD) is required to provide high-resolution insights into the crystallographic structure, strain effects produced by doping and phase purity of the material. The larger intensity and high resolution of synchrotron XPD will allow a more precise understanding of the structural modifications in the doped films, which is crucial for optimizing their dielectric properties.

These findings reveal that the controlled doping (time dependent) of ZnO nanoparticles with rare-earth and transition metal elements can significantly change their dielectric properties, making them an ideal candidate for next-generation transparent electronic applications, including high-performance CDC-based devices.

References

[1] H. Wanbiao, et al. *Electron-pinned defect-dipoles for high-performance colossal permittivity materials*. Nature Materials 12, 821-826 (2013).

[2] I. Sidra, et al. *Realistic dielectric response of high temperature sintered ZnO ceramic: a microscopic and spectroscopic approach.* RSC Advances 10, 30451-30462 (2020).

[P1.30] Structure and Electronic Properties of Al-doped ZnO and Niobium Oxides

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The development of materials with high solar energy harvesting and conversion efficiency is essential for a sustainable future. Oxide thin films, particularly Al-doped ZnO (AZO) and niobium oxides (Nb_2O_5 and NbO_2), are highly promising due to their tunable optoelectronic and structural properties. These materials have broad applications in transparent electronics, photocatalysis, energy storage, and photovoltaics. In this study, we systematically investigate them in structure and electronic properties.

For AZO thin films, we achieve low electrical resistivity by inducing structural disorder and varying Al doping during the growth process, resulting in an amorphous phase [1]. Amorphous conducting films offer advantages such as an enhanced percolation network for carrier transport and improved mechanical stability. To understand the impact of reduced structural order, we correlate amorphization with electronic properties using HAXPES, Hall, and optical measurements. Our analysis reveals a significant increase in the density of states near the Fermi level in amorphous AZO compared to polycrystalline AZO, along with notable valence band modifications.

In the case of Niobium Oxides, we develop a novel growth process to obtain its multiple phases (NbO, NbO_2, and Nb_2O_5). These films are characterized using XRD, XPS, and UV-Vis spectrophotometry. Additionally, X-ray absorption near-edge spectroscopy at the Nb K-edge, performed with X-ray free-electron laser radiation, provides insights into the electronic structure and bulk stoichiometry of the films [2].

Our findings contribute to the understanding and advancement of oxide thin films for next-generation energy applications.

References

[1] R. Magrin Maffei, et al. *Defectivity of Al:ZnO thin films with different crystalline order probed by Positron Annihilation Spectroscopy.* Appl. Surf. Sci. 665, 160240 (2024).

[2] S. Pelatti, et al. *Niobium oxide films with variable stoichiometry: structure, morphology and ultrafast dynamics*, J. Phys. Chem. C. In press (2025).

[P1.31] Development of Reverse MonteCarlo approach for Generation of Metallic Glass Structures with Minimal Cells

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Bulk Metallic Glasses are amorphous materials that display unique electronic and mechanical properties. The exploration of their properties through atomistic approaches requires the generation of realistic structures able to capture both the short-range order (SRO) and medium-range order (MRO) features, correctly. This may correspond to large geometrical models with thousands of atoms. Such large simulations cells imply huge computational costs and prevent their use, e.g., in first principles investigations, that are usually limited to a few hundreds of atoms per cell. In this work, we developed a new numerical approach based on Reverse Monte Carlo (RMC) scheme to construct reliable metallic glass structures with the smallest number of atoms, yet preserving the correct SRO and MRO of larger structures. In the case of CuZr – the archetype of – our approach provides minimal amorphous models with only 32 atoms per cell [1] that well reproduce the structural and electronic properties of reference systems with ~10000 atoms.

Reference

[1] B. I. Adetunji, et al. submitted (2025).

[P1.32] Ab initio DFT calculations of thermoelectric properties of InAs-InAsSb nanowire heterostructures, speeded up by Machine Learning

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We present initial results on a computational study on the thermoelectric and transport properties of various InAs-InAsSb nanowire heterostructures, particularly those formed by twinning planes along their growth direction and by the junction between InAs-wurtzite) and InAsSb-zincblende phases. The related experimental results were displayed in [1], which demonstrates how the inclusion of twinning planes in nanowires can reduce only the lattice thermal conductivity of the material while keeping electronic transport unchanged, leading to an increase in the figure of merit. In this project, Density Functional Theory (DFT) formalism implemented in the Quantum Espresso suite of codes [2] and combined with Wannier functions [3] has been used to solve the Boltzmann Transport Equation as implemented in the Phoebe code [4] for both electrons and phonons, to simulate the transport properties of such nanostructures. It has been shown that Wannier transport calculations (DFT+Wannier functions+BTE) can accurately predict the thermoelectric figure of merit of these pure phase nanowires, considering only the electron-phonon scattering mechanisms, which are dominant for these systems near room temperature. With this framework, it is possible to simulate, entirely from first principles, the full transport properties for varying temperatures and doping concentrations within the rigid band approximation, also accounting for isotopic scattering and dimensionality effects, thus demonstrating the power of ab initio simulations applied to these nanostructures, where the experimental measurement processes are not trivial. Fig. 1 presents the calculated ZT results for InAs ZB, WZ and the twinned superlattice nanowire (TSLNW) phases, which are in very good agreement with the experimental values. Furthermore, a Machine Learning (ML) technique, as implemented in the hiPhive code [2], was used to speed up the calculation of third order force constants necessary to evaluate the lattice thermal conductivity, which is the main bottleneck of the entire ZT computation. Using ML regression algorithms an incredible speedup was achieved for the calculation of third-order force constants, drastically reducing the number of DFT calculations needed for the computation of the phonon-phonon interaction [3].

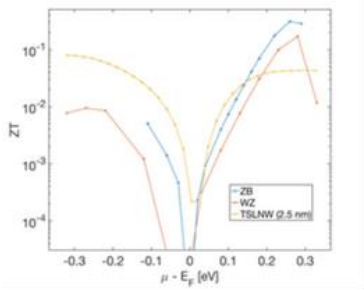

Figure 1. Figure of merit of InAs zincblend (ZB), wurtzite (WZ) and twinned superlattice nanowire with 2.5 nm

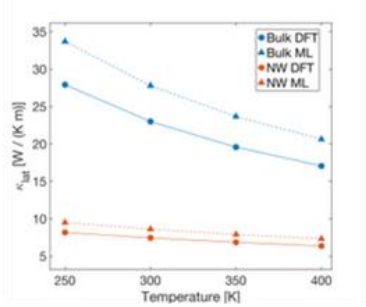

Figure 2. Lattice thermal conductivity calculated with the full sqaicall approach (labeled DFT) and with

References
[1] L. Peri, et al. Nano Energy 103, 107700 (2022).
[2] P. Giannozzi, et al. The Journal of Chemical Physics 152 (2020).
[3] A. A. Mostofi, et al. Computer physics communications 178, 685-699 (2008).
[4] A. Cepellotti, et al. Journal of Physics: Materials 5, 035003 (2022).
[5] F. Eriksson, E. Fransson, and P. Erhart. Advanced Theory and Simulations 2, 1800184 (2019).

[P1.33] First-principles study of bound excitons in monolayer SnS2

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SnS2 is a layered material with visible spectrum absorption and energy level alignment suitable for hydrogen fuel cell electrodes [1]. It exemplifies group-IV chalcogenides, increasingly studied for second harmonic generation (SHG) response [2]. We undertake a thorough theoretical investigation of bound excitons in monolayer SnS2, employing many-body perturbation theory [3] on top of DFT-PBE electronic structure calculations [4]. Our study reveals a richer structure of bound excitons than previously reported [5], likely due to overscreening from the interlayer interaction in the previous work. The calculated first bright-exciton energy of 2.3 eV closely matches the experimental optical gap of 2.23 eV. We offer a detailed analysis of the composition and nature of the excitonic states. Future research will extend to non-centrosymmetric group-IV chalcogenide systems such as SnS and SnSe layered systems, also exploring their SHG response [6].

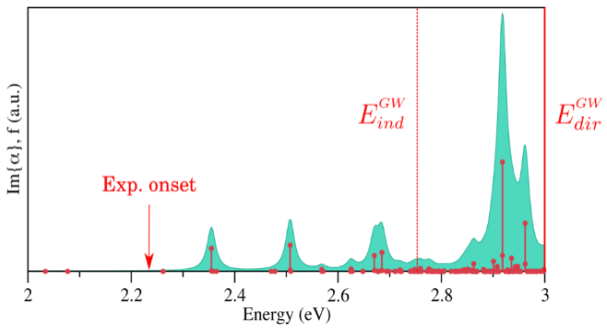

Fig. 1: BSE optical response of monolayer SnS2 for in-plane electric-field polarization: red dots and bars indicate the optical excitation energies and associated oscillator strengths, the light-green curve is the imaginary part of the 2D polarizability, and the vertical lines indicate the direct and indirect GW band gaps. The experimental absorption onset was taken from [1].

References

[1] Y. Sun, et al. *Freestanding tin disulfide single-layers realizing efficient visible-light water splitting*. Angew. Chem. Int. Ed. 51, 8727 (2012).

[2] H. Wang and X. Qian. *Giant optical second harmonic generation in two-dimensional multiferroics.* Nano Lett. 17, 5027 (2017).

[3] D. Sangalli, et al. *Many-body perturbation theory calculations using the Yambo code*, J. Phys. Condens. Matter. 31, 325902 (2019).

[4] A. Marini, et al. *Yambo: an ab initio tool for excited state calculations.* Comput. Phys. Commun. 180, 1392 (2009).

[5] J. P. Perdew, K. Burke, and M. Ernzerhof. *Generalized gradient approximation made simple.* Phys. Rev. Lett. 77, 3865 (1996).

[6] P. Giannozzi, et al. Advanced *capabilities for materials modelling with Quantum Espresso.* J. Phys. Condens. Matter. 29, 465901 (2017).

[7] H. L. Zhuang and R. G. Hennig. *Theoretical perspective of photocatalytic properties of single-layer SnS2.* Phys. Rev. B 88, 115314 (2013).

[8] E. Luppi, et al. *Ab initio second-order nonlinear optics in solids: Second-harmonic generation spectroscopy from time-dependent density-functional theory.* Phys. Rev. B 82, 235201 (2010).

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[P1.34] Charge Transfer and Hybrid States in Inverted-Gap Core-Shell Nanowires

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Nanowires are rising much interest as a novel nanoelectronic platform for light harvesting, controlled single- or few-photon emitters, and for the realization of topological states e.g. Nanowires are rising much interest as a novel nanoelectronic platform for light harvesting, controlled single- or few-photon emitters, and for the realization of topological states, e.g., in superconductor proximitized nanostructures. Core-shell nanowires, adding one or more radial layers of a different material to a central nanowire core, expand substantially the possibility to engineer the bandstructure, by tuning the geometric parameters of the sample, its doping profile, and the type of band alignment between different materials [1]. In case the radial hetherojunction presents a type-2 inverted-gap alignment [2], electron and hole states coexist at the same energy, and the hybridization of these states takes place. The mesoscopic modeling of such structures is very challenging, as both types of carriers must be considered at energies inside the broken gap.

We present our investigation on the electronic structure of InAs-GaSb core-shell nanowires using a self-consistent, 8-band k.p approach which considers the symmetry and crystallographic directions of the nano-crystal, its realistic hexagonal section and, possibly, external electric fields. Our method, aimed at reproducing the expected charge transfer effects, is based on a real-space finite-element solution resulting in a very efficient approach.

In particular, we are interested in the fundamental band gap of the system (Fig. 1, left), the hybridization gap which results from anticrossing of the inverted electron and hole subbands. We will illustrate the charge transfer at the interface and how we include such self-consistent effects. Specifically, we extended and implemented approaches previously proposed in the context of InAs-GaSb quantum wells, exposing the substantial effect of the corresponding built-in electric field on the fundamental band gap of the system, which were neglected in previous investigations [3]. We will show how the inclusion of self-consistent electrostatic effects is essential to predict the system parameters at which the effective energy gap vanishes and the formation of topological end states [4].

References

[1] A. Vezzosi, A. Bertoni, and G. Goldoni. *Band structure of n - and p -doped core-shell nanowires.* Phys. Rev. B 105, 245303 (2022).

[2] V. Clericò, et al. *Spin-Resolved Magneto-Tunneling and Giant Anisotropic g-Factor in Broken Gap InAs-GaSb Core-Shell Nanowires*. Nano Letters 24, 790 (2024).

[3] N. Luo, et al. *Band-inverted gaps in InAs/GaSb and GaSb/InAs core-shell nanowires*. Scientific Reports 6, 38698 (2016).

[4] A. Vezzosi, A. Bertoni, M. Gibertini, and G. Goldoni. Submitted (2025).

[P1.35] A coarse grained model for Amyloid Beta aggregation: enhancing structural accuracy using atomistic simulations

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The aggregation process of amyloid beta (Aβ) protein, believed to be at the basis of Alzheimer's disease, seems to be triggered by a transition from a disordered to an aggregation-prone state [1]. However, the features of this aggregation-prone conformation, the aggregation pathway and the structure of intermediate aggregates remain poorly understood [2]. Atomistic simulations provide insights into early aggregation but are limited by computational constraints [3]. Coarse-grained (CG) models offer a solution, but existing ones either have high computational costs [4] or compromise accuracy [5]. To address this, we have constructed a minimalist single-bead-per-amino-acid CG model of the Aβ, parametrized using an extensive dataset of atomistic simulations. This dataset, obtained using different force fields optimized for disordered proteins [3] and validated against experimental data, includes both non-aggregation-prone and aggregation-prone conformations (Fig. 1 (a)) [6]. The latter were identified through flexible docking and exhibit a β-sheet-rich hydrophobic core and a beta-hairpin structure, consistent with fibril data. We have optimized the bonded terms of the CG model to preserve these features and derived non-bonded interactions from the CALVADOS force field [7], previously validated for GFP aggregation [8].
This accurate and predictive CG model will enable studies on Aβ aggregation (Fig.1 (b)) under different environmental conditions and the influence of nanomaterials.

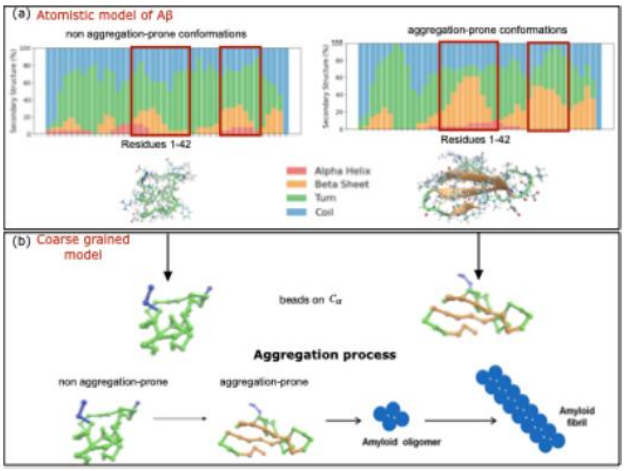

Fig. 1: (a) Secondary structure percentage for each residue of Aβ in aggregation-prone and non-aggregation-prone conformations, obtained from atomistic simulations. (b) Mapping to the coarse-grained model for different configurations and schematic representation of the aggregation process, which can be simulated using the coarse-grained model.

References

[1] M.G. Iadanza, et al. Nat. Rev. Mol. Cell Biol. 19, 755 (2018).
[2] M. Carballo-Pacheco and B. Strodel. J. Phys. Chem. B 120, 2991 (2016).
[3] S. Paul, et al. Phys. Chem. Chem. Phys. 12, 6652 (2020).
[4] J. Maupetit, et al. *A coarse-grained protein force field for folding and structure prediction.* Proteins 69, 394 (2007).
[5] M. Cheon, I. Chang, and C.K. Hall. Proteins 78, 2950 (2010).
[6] M. Bini, V. Tozzini, and B. Luca. *Structural characterization of β-Amyloid monomer in solution. I*n preparation.
[7] G. Tesei and K. Lindorff-Larsen. Open Res. Eur. 2, 94 (2023).
[8] M. Bini and V. Tozzini. Macromolecules. In preparation.

[P1.36] Pressure-Induced Phase Transition and Thermal Transport Properties of CrTe: An Ab-Initio Study

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In this study, we investigate the thermal transport properties of chromium telluride (CrTe) in its ground-state and across pressure-induced phase transitions [1] using ab-initio density functional theory (DFT). We analyze the stability of different crystalline phases under varying pressure conditions, identifying structural and magnetic transitions that significantly influence the electronic band structure and thermal transport behavior [2]. Our results show that pressure alters the magnetic ordering and modifies the phonon scattering mechanisms, leading to notable changes in thermal conductivity. The complex interplay between structural, magnetic, and electronic properties under pressure is explored, providing insight into the fundamental mechanisms governing thermal transport in CrTe. This work underscores the potential of pressure as a tuning parameter for optimizing the thermal and magnetic properties of CrTe for thermoelectric and spintronic applications.

References

[1] V. Kanchana, G. Vaitheeswaran, and M. Rajagopalan. *Pressure-induced structural and magnetic phase transition in ferromagnetic CrTe.* Journal of magnetism and magnetic materials 250, 353-363 (2002).
[2] T. Eto, M. Ishizuka, S. Endo, T. Kanomata, and T. Kikegawa. *Pressure-induced structural phase transition in a ferromagnet CrTe.* Journal of alloys and compounds 315, 16-21 (2001).

[P1.37] Defect complexes and charge compensation in Ta-doped anatase TiO_2 transparent conductor

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Functional materials are at the heart of technological advancements. Among them, transparent conductive oxides (TCOs) combine low electrical resistivity, typical of metals, and high transparency in the visible region, typical of insulators [1]. For this unique characteristic, TCOs are of particular interest for optoelectronic applications spanning from photovoltaic solar cells to plasmonics, and flexible and smart devices.

The stability and behavior of point defects and defect complexes in Ta-doped anatase TiO_2 (TaTO) TCO and their effect on its structural, electronic, optical, and transport properties are comprehensively investigated [2] using state-of-the-art first principles simulations based on DFT and experimental measurements under various synthesis conditions. Oxygen vacancies (V_O) and titanium interstitials (Ti_I), which readily form under O-poor conditions, act as intrinsic shallow donors that promote n-type conductivity alongside extrinsic tantalum doping (Ta_{Ti}). While clustering of intrinsic donor defects is irrelevant both energetically and electronically, Ta clustering is inhibited. In contrast, O interstitials (O_I) and, particularly, Ti vacancies (V_{Ti}), which form more easily under O-rich conditions, introduce gap states and behave as deep acceptors, strongly compensating the effect of shallow extrinsic donors. In this scenario, intrinsic acceptors and Ta donors preferentially form neighboring configurations. The interactions between dopants and multiple native defects introduce nonlinear charge-compensation effects, which can reduce the quasi-free charge carriers even in presence of significantly high levels of extrinsic donor doping ($N_D = 10^{20}$–10^{21} cm^{-3}). This mitigates visible transmittance loss while sustaining and fine-tuning TC properties. Theoretical predictions and experimental evidence confirm that anatase TiO_2-based TCOs: (i) necessitate O-poor synthesis conditions or high concentrations of donor defects to maintain low resistivities; and that (ii) in O-poor conditions, V_O primarily contributes to the transmittance loss in the visible range. Overall, this study provides valuable insights into the properties of anatase TiO_2 and TaTO as well as defect engineering strategies to optimize these materials for applications in transparent electronics and optoelectronic devices.

References

[1] S. C. Dixon, D. O. Scanlon, C. J. Carmalt, and I. P. Parkin. *n-Type doped transparent conducting binary oxides: an overview.* J. Mater. Chem. C 4-29, 6946–6961 (2016).

[2] L. Bursi, A. Catellani, P. Mazzolini, C. Mancarella, A. Li Bassi, A. Baraldi, and A. Calzolari. *Defect complexes and charge compensation in Ta-doped anatase TiO_2 transparent conductor.* Submitted.

[P1.38] Tailorable materials for plasmonics in extreme conditions

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Discovering multifunctional materials with tunable plasmonic properties, capable of surviving harsh environments is critical for advanced optical, photothermal, and telecommunication applications. By using ab initio simulations based on (TD)DFT, we first studied the role of composition and structural disorder of transition-metal nitrides [1-3], and we provided an efficient strategy to engineering stable, easy-to-grow hyperbolic metamaterials, with extraordinary mechanical properties [4]. Finally, by combining computational thermodynamics and first principles electronic structure techniques [5], we proposed high-entropy transition-metal carbides [6], which yielded plasmonic properties from room temperature to 1500K (Fig. 1). This new class of plasmonic materials may foster previously unexplored optical/mechanical applications (e.g., aerospace and security systems) in extreme conditions and ultra-high temperature.

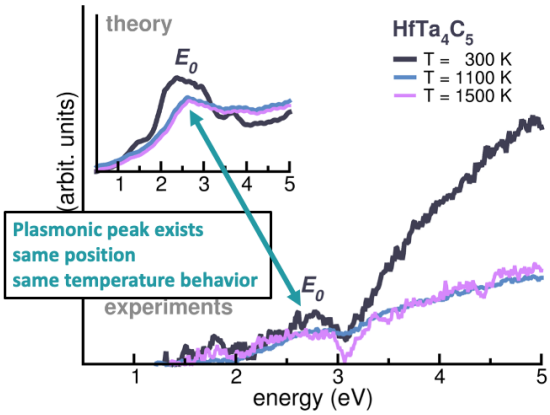

Fig. 1: Comparison between experimental and theoretical (inset) EELS spectra of high entropy $HfTa_4C_5$ as a function of temperature. Image adapted from Ref. [6].

References

[1] A. Catellani and A. Calzolari. *Plasmonic properties of refractory titanium nitride.* PRB 95, 115145 (2017).

[2] D. Shah, A. Catellani, H. Reddy, N. Kinsey, V. Shalaev, A. Boltasseva, and A. Calzolari. *Controlling the Plasmonic Properties of Ultrathin TiN Films at the Atomic Level.* ACS Phot. 5, 2816 (2018).

[3] A. Catellani, P. D'Amico, and A. Calzolari. *Tailoring the plasmonic properties of metals: The case of substoichiometric titanium nitride*. PRMater. 4, 015201 (2020).

[4] A. Calzolari, A. Catellani, M. Buongiorno Nardelli, and M. Fornari. *Hyperbolic Metamaterials with Extreme Mechanical Hardness*. Adv. Opt. Mater. 9, 2001904 (2021).

[5] S. Divilov, et al. *Disordered enthalpy–entropy descriptor for high-entropy ceramics discovery*. Nature 625, 66 (2024).

[6] A. Calzolari, C. Oses, C. Toher, M. Esters, X. Campilongo, S. P. Stepanoff, D. E. Wolfe, and S. Curtarolo. *Plasmonic high-entropy carbides*. Nature Commun. 13, 5993 (2022).

[P1.39] Conformational heterogeneity and protonation equilibria shape the photocycle branching in channelrhodopsin-2

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The emerging field of optogenetics exploits the genetic encoding of photoactive proteins to control physiological processes with high spatiotemporal resolution and in a wavelength-dependent manner. Microbial rhodopsins serve as primary optogenetic tools due to their ability to regulate neuronal activity via light-gated ion channels or light-driven pumps. Channelrhodopsin-2 (ChR2) is the most used optogenetic tool and a widely investigated rhodopsin. Upon light absorption, the retinal cofactor undergoes photoisomerization from the all-trans (D470 state) to the 13-cis configuration (P500 state). This conformational change induces the flow of water and ions through the channel on the microsecond timescale, followed by the recovery of the closed resting state within milliseconds. However, despite extensive experimental studies, many structural modifications associated with photocycle intermediates remain debated [1]. Of particular interest is the localization of the P480 intermediate within the photocycle, which may involve a C=N anti/syn isomerization, as well as the timing of the deprotonation of glutamic acid E90, a critical residue for ChR2 function. In this study, we investigate the possibility of an early-P480 state, formed directly upon photoillumination of the dark-adapted state, in which E90 is deprotonated, as hypothesized in a previous work [2]. Employing extended molecular dynamics simulations and QM/MM multiscale calculation based on the Perturbed Matrix Method [3], we computed the deprotonation free energy, and the infrared band associated with E90, supporting the existence of the early P480 state [4]. Our findings also show that the protonation state of E90 is influenced by diverse interconnected variables and provide molecular insights linking E90's interaction pattern with its deprotonation propensity. Specifically, our data demonstrate that both protonated and deprotonated E90 states are possible in P480, depending on E90's hydrogen bonding pattern, explaining the molecular mechanism underlying P480 accumulation under continuous illumination. By establishing robust correlations between structural changes and infrared spectral features in ChR2, our findings refine the interpretation of experimental data. This work is expected to enhance our understanding of the molecular mechanisms underlying optogenetic control, ultimately improving the precision and effectiveness of such tools in neuroscience and beyond.

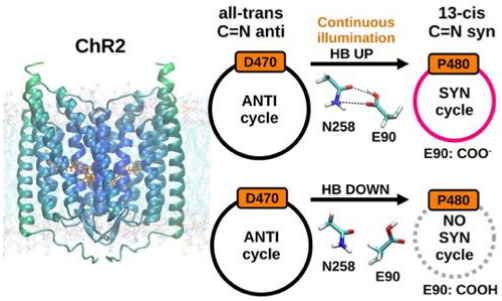

Fig. 1: Schematic representation of the Channelrhodopsin2 membrane protein and the photocycle branching induced by variations in the hydrogen-bond network involving the Glu90 residue.

References

[1] V. A. Lórenz-Fonfría and J. Heberle. (BBA)-Bioenergetics, 1837(5), 626-642 (2014).
[2] J. Kuhne, et al. Proc. Nat. Acad. Sci. 116(19), 9380-9389 (2019).
[3] L. Zanetti-Polzi, et al. Phys. Chem. Chem. Phys. 20(37), 24369-24378 (2018).
[4] L. Bellucci, M. Capone, I. Daidone, and L. Zanetti-Polzi. J. Bio. Macromol. 305, 140977 (2025).

[P1.40] A Machine Learning approach targeting the screened potential of 2D materials in the GW approximation

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This work addresses the computational challenges of achieving convergence (notably with respect to the kinetic energy cutoff used to represent the response functions) in GW calculations for 2D materials [1], by introducing a machine learning (ML)-based approach to accelerate calculations of response functions and, subsequently, quasi-particle corrections. Specifically, convolutional neural networks (CNNs) are employed to predict high-energy cut-off properties from lower-energy inputs. CNNs are trained to infer missing data, effectively reconstructing high-cutoff response functions with reduced computational cost, as compared to explicit calculations. Initial tests on materials like h-BN, MoS2, and phosphorene demonstrate that CNNs can identify and extrapolate patterns in the response functions associated with these materials (Fig.1). The methodology focuses on slices of response tensors (X), represented as images, which CNNs process to enhance the X energy cut-offs, possibly incrementally. More advanced architectures of the models are under investigation to improve on the generalization of the networks [3, 4].
The integration of this kind of ML tools into suites like YAMBO [2] promises to significantly reduce the time and cost of Green's function-based electronic structure calculations, paving the way for advancements in materials design and discovery, by accelerating the convergence of the screened Coulomb potential of 2D materials, moving towards more complete and complex simulations of electronic and optical properties.

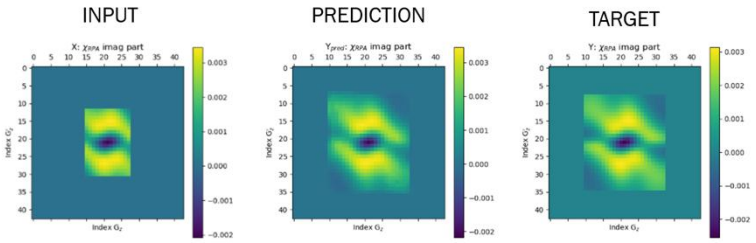

Fig. 1: Example of performance on hBN RPA response slices, trained on hBN independent-particle ones, where X is the input image (4 Ry), Y the target output (8 Ry) and Ypred the prediction.

References

[1] D. Golze, M. Dvorak, and P. Rinke. *The GW Compendium: A Practical Guide to Theoretical Photoemission Spectroscopy.* Front. Chem. 7, 377 (2019).
[2] D. Sangalli, et al. *Many-body perturbation theory calculations using the yambo code.* J. Phys.: Condens. Matter 31, 325902 (2019).
[3] J. Schmidt, M.R.G. Marques, S. Botti, et al. *Recent advances and applications of machine learning in solid-state materials science.* npj Comput Mater 5, 83 (2019).
[4] B. Lu, Y. Xia, Y. Ren, M. Xie, L. Zhou, G. Vinai, S. A. Morton, A.T.S. Wee, W. G. van der Wiel, W. Zhang, and P.K.J. Wong. *When Machine Learning Meets 2D Materials: A Review*. Adv. Sci. 11, 2305277 (2024).

[P1.41] Excitons in bilayer WTe_2

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Bilayer WTe_2 is a remarkable two-dimensional metal, since it exhibits a macroscopic out-of-plane electric dipole despite the presence of charge carriers that screen the electrostatic forces between ions [1].
At low temperature the system develops a narrow transport gap, like its monolayer counterpart where the appearance of the gap has been attributed to condensation of excitons [2]. The similarities between transport measurements in mono and bilayer structures suggest that similar excitonic physics is at play in the bilayer.
Contrary to other known bilayer excitonic insulators, in which electrons and holes are spatially separated, in WTe_2 interlayer tunneling is significant. This might impact the observable features of the putative exciton condensate, giving rise to a coherent contribution to the ferroelectric dipole.
In this work we investigate bilayer WTe_2 both from first principles and using a model that builds upon the symmetries of the system. We focus on excitons derived from a model Bethe-Salpeter equation. The goal is to assess the instability against exciton condensation, as well as to predict its possible experimental fingerprint.

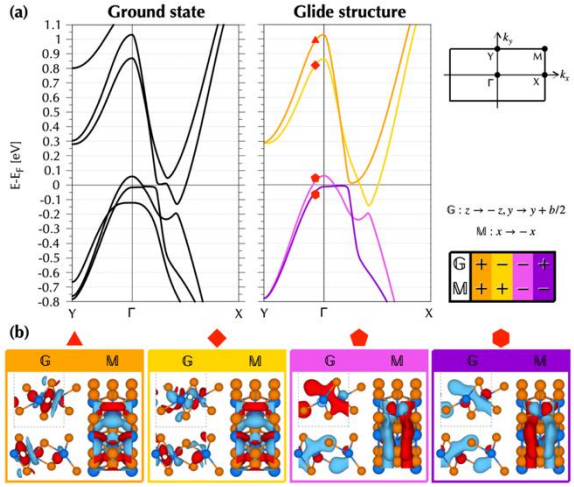

Fig. 1: (a) DFT-PBE bands of bilayer WTe_2: ground state structure (left) and structure with glide symmetry (right). Brillouin zone in the top right corner. (b) Real part of Kohn-Sham wavefunctions at k points marked by red shapes. The side and top views show the sign of the states with respect to the glide (G) and mirror (M) symmetry, as reported in the table.

References

[1] Z. Fei, W. Zhao, T. A. Palomaki, B. Sun, M. K. Miller, Z. Zhao, J. Yan, X. Xu, and D. H. Cobden. *Ferroelectric switching of a two-dimensional metal.* Nature 560, 336-339 (2018).
[2] B. Sun, W. Zhao, T. A. Palomaki, et al. *Evidence for equilibrium exciton condensation in monolayer WTe_2.* Nature Physics 18, 94-99 (2022).

[P1.42] Coupling Many Body Perturbation Theory with Polarizable Continuum Models

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The theoretical description of quantum systems embedded in external environments represents a challenge for what concerns the application of Many Body Perturturbation Theory (MBPT) approaches to the study of the electronic excitations.
Different levels of accuracy can be used to treat the actual system, for which a quantum mechanical description is employed, and its surrounding environment, that can be approximated through a simplified quantum mode, a molecular mechanical approach, or a continuum model.
In this contribution we will present a theoretical framework in which the MBPT treatment of the quantum system is coupled to a Polarizable Continuum Model description of its surrounding environment. The formalism has been implemented within the YAMBO platform [1, 2] by exploiting the ENVIRON package [3] available withing the QuantumEspresso suite of codes [4, 5].
We will present results obtained with the developed methodology for a selected class of systems.

References

[1] A. Marini, C. Hogan, M. Grüning, and D. Varsano. Y*ambo: An ab initio tool for excited state calculations.* Comp. Phys. Commun. 180, 1392 (2009).
[2] D. Sangalli, et al. *Many-body perturbation theory calculations using the yambo code.* J. Phys. Cond. Mat. 31, 325902 (2019).
[3] O. Andreussi, I. Dabo, and N. Marzari. R*evised self-consistent continuum solvation in electronic-structure calculations.* J. Chem. Phys. 136, 064102 (2012).
[4] P. Giannozzi, et al. *QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials.* J. Phys. Cond. Mat. 21, 395502 (2009).
[5] P. Giannozzi, et al. *Advanced capabilities for materials modelling with Quantum ESPRESSO.* J. Phys. Cond. Mat. 29, 465901 (2017).

[P1.43] Modeling Electronic Excitations in Photoswitch/Quantum Dot Systems: A Study of Photoisomerization in Functionalized Azobenzene

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The functionalization of molecular photoswitches (PhSs) with semiconductor quantum dots (QDs) into nanohybrids enables enhanced electronic and optical properties. These Photoswitch-Quantum Dot (PhS+QD) systems are particularly promising for applications in biomedicine, catalysis, and sensing [1]. However, a key challenge in understanding their functionality lies in accurately modeling electronic excitations during the photoisomerization of the photoswitch, especially when achieving resonance with the quantum dot, as computational complexity increases exponentially with QD size [2]. Conventional computational approaches often neglect crucial electron correlation effects, limiting their ability to describe intricate photochemical phenomena such as conical intersections and avoided crossings [3]. To address this, we investigate the electronic structure of functionalized azobenzene (AB) coupled to cadmium selenide quantum dots (CdSeQDs) using Hybrid Configuration Interaction (HyCI), a methodology for nanohybrids that integrates correlated electronic structure methods to achieve a balance between accuracy and computational feasibility. We provide a detailed characterization of the hybrid Potential Energy Surface (see Fig. 1 below) along the primary photoisomerization coordinate, including the conical intersection of AB. Our analysis of different optical features reveals the emergence of two asymmetrical avoided crossings at resonance when CdSeQDs exceed 4 nm in size, leading to an energy splitting of approximately 5 meV. This splitting, combined with the picosecond-scale lifetime of optical electronic excitations, may influence the efficiency of photoisomerization. These findings offer new insights into the complex electronic interactions governing PhS+QD nanohybrids, highlighting their potential for controlled photochemical switching. Future work will focus on reaction quantum yields and dynamic pathways using non-adiabatic molecular dynamics simulations.

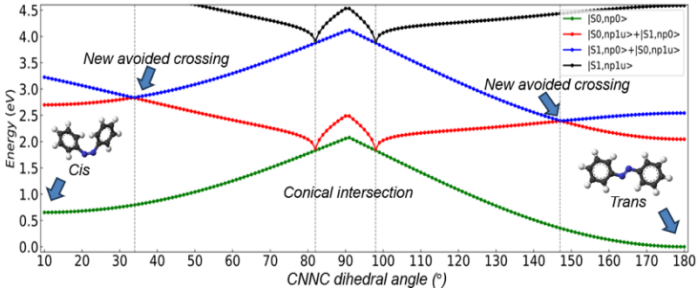

Fig. 1: Potential Energy Surface of Azobenzene + CdSeQD with respect to its primary reaction coordinate.

References

[1] C. Fedele, T. P. Ruoko, K. Kuntze, M. Virkki, and A. Priimägi. *New tricks and emerging applications from contemporary azobenzene research*. Photochem Photobiol Sci 21, 1719–1734 (2022).

[2] G. Gil, S. Corni, A. Delgado, A. Bertoni, and G. Goldoni. *Excitation energy-transfer in functionalized nanoparticles: Going beyond the Förster approach*. J. Chem. Phys. 144, 074101 (2016).

[3] J. Fregoni, G. Granucci, E. Coccia, M. Persico, and S. Corni. *Manipulating azobenzene photoisomerization through strong light–molecule coupling*. Nat Commun 9, 4688 (2018).

[P1.44] Structural and dynamic effects of S-nitrosation on a Blue Fluorescent Protein

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S-nitrosation of cysteine residues, whereby a nitroso group is added to the cysteine sulfur atom, is a key post-translational modification that can modulate protein structure and function. In the case of the blue fluorescent protein mTagBFP2, S-nitrosation has been shown to significantly quench fluorescence (by around 70%), making it a promising intracellular nitric oxide (NO) sensor. Mutagenesis and mass spectrometry experiments have demonstrated that two key cysteine residues contribute to the reduction in fluorescence quantum yield and lifetime upon NO exposure [1]. Förster Resonance Energy Transfer (FRET) from the mTagBFP2 chromophore to the S-nitroso group was shown to account for a large part of the quenching [2]. However, particularly in the case of one of the two cysteine residue, FRET does not fully explain the observed fluorescence loss. To explore alternative quenching mechanisms, we performed molecular simulations to compare the structural dynamics of nitrosated and non-nitrosated mTagBFP2. By analyzing tunnel formation and NO diffusion pathways, we assessed whether the NO radical can reach the chromophore through transiently opening channels, thereby quenching its fluorescence. Additionally, we examined root mean square fluctuations (RMSF) and key inter-residue distances to evaluate structural perturbations caused by S-nitrosation. Our results suggest that a combination of NO diffusion and conformational changes may contribute to the additional fluorescence quenching, providing a more comprehensive understanding of the effects of S-nitrosation on mTagBFP2.

References

[1] C. Montali, S. Abbruzzetti, A. Franzen, G. Casini, S. Bruno, P. Delcanale, S. Burgstaller, J. Ramadani-Muja, R. Malli, T. Gensch, and C. Viappiani. *Nitric Oxide Sensing by a Blue Fluorescent Protein*. Antioxidants 11-11, 2229 (2022).
[2] *Intramolecular Energy Transfer to S-nitrosated Cys residues is at the basis of fluorescence sensitivity to nitric oxide in a fluorescent protein.* In preparation.

[P1.45] Pressure and Magnetic Field Control of the Topological Phase In Antiferromagnetic Bilayers

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Antiferromagnetic bilayers are said to be A-type when spins align ferromagnetically within each layer but point in opposite directions in the two layers, resulting in a zero net magnetization. The opposite orientation of majority spins in the two layers strongly suppresses interlayer hopping and the electronic structure is not affected significantly by a change in interlayer distance. Nonetheless, an external magnetic field can drive a metamagnetic transition into a fully ferromagnetic state, where spins in both layers are parallel, so that interlayer hopping is possible and energy bands are sensitive to the separation between the layers. This difference can be exploited to manipulate the energy bands of an A-type antiferromagnetic bilayer by means of the combined effect of pressure and magnetic field. Here we consider bilayer CrSBr as a prototypical example and show using first-principles simulations that pressure affects the interlayer distance, enhancing the interlayer hopping in the ferromagnetic state, and eventually closes the energy gap, inducing a topological phase transition. Remarkably, depending on the magnetization direction it is possible to tune the system either in a quantum anomalous Hall insulating state when spins are out-of-plane or into a half Chern-Weyl semimetallic phase when spins are in-plane, with the emergence in both cases of topological edge states. We expect this phenomenon to be general to A-type antiferromagnetic bilayers, opening interesting perspectives on the manipulation of their topological character towards applications in spintronics and quantum computation.

Project
PNRR-M4C2INV1.5, NextGenerationEU-Avviso 3277/2021-ECS 00000033-ECOSISTER-spok6.PNRR-M4C2INV1.5, NextGeneration EU. Avviso 3277/2021-ECS 00000033-ECOSISTER-spoke 6.

[P1.46] Ionic liquid at gold surface

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Room Temperature Ionic Liquids (RTIL) are very promising materials as electrolytes for applications in energy storage and in many fields of nanoelectronics and spintronics. Moreover, they are ideal candidates for a green and sustainable technology due to low melting point, low volatility, and high thermic stability. To understand and exploit these potentialities it is crucial to clarify the electric double layer consisting in a multilayer structure of cations and anions observed in the region of the liquids near a metallic surface, and its modifications when an electric field is present.

In this paper we report the results of a systematic investigation performed by means of molecular mechanics simulations of the electrical double layer of a RTIL composed by the cation EMIM and the anion NTf_2 embedded between two gold surfaces. We have evaluated the mass and charge densities of the ions near the interfaces and in the central bulk region, comparing the results obtained in the cases of neutral and oppositely charged surfaces to follow the evolution of the structure and the composition of the layers. To have a more complete description of the system, we have also calculated the vibrational spectra of cations and anions in the same regions to have an indication of the electrostatic interactions existing near the surfaces.

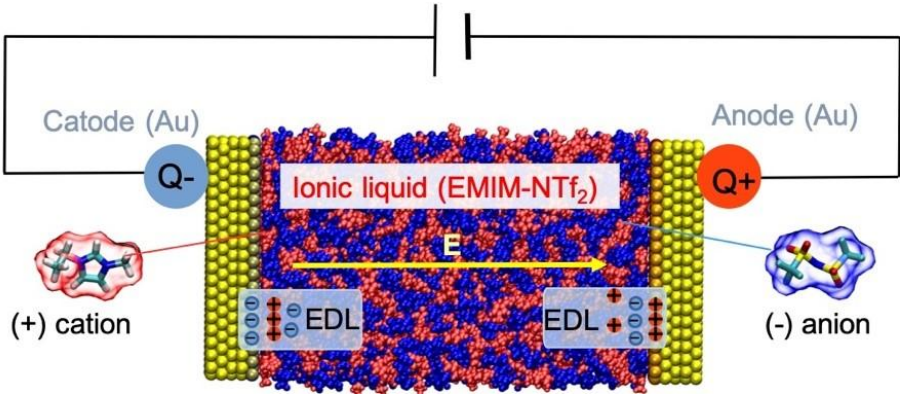

Fig. 1: schematic representation of the room temperature ionic liquid studied, composed by the cation EMIM and the anion NTf_2 embedded between two neutral or charged gold surfaces. The electrical double layer (EDL) formed near the interfaces is indicated.

[P1.47] Functional Theory of the Occupied Spectral Density

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We address the problem of interacting electrons [1] in an external potential by introducing the occupied spectral density as fundamental variable [2]. First, we formulate the problem using an embedding framework [3] and prove a one-to-one correspondence between a spectral density and the local, dynamical external potential that embeds it into an open quantum system. Then, we use the Klein functional to (*i*) define a universal functional of the spectral density, (*ii*) introduce a variational principle for the total energy, and (*iii*) formulate a non-interacting mapping suitable for numerical applications.
The resulting equations [2], which involve local and dynamical potentials, are then solved by using the algorithmic inversion method [3,4,5,6] based on a sum-over-poles to represent propagators. At variance with time-dependent density-functional theory, this formulation aims at studying charged excitations and electronic spectra with a functional theory, although an explicit and formally correct description of all electronic levels could also lead more naturally to accurate approximations for the total energy.

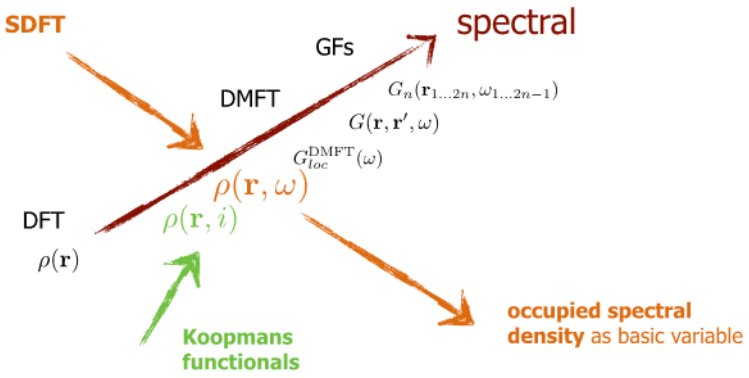

Fig. 1: Climbing the hierarchy of spectral electronic-structure methods: From the charge density to the spectral density as basic variable.

References

[1] N. Marzari, A. Ferretti, and C. Wolverton. *Electronic-structure methods for materials design.* Nature Materials 20, 736 (2021).
[2] A. Ferretti and N. Marzari. *Functional theory of the occupied spectral density.* Preprint. (2025).
[3] A. Ferretti, T. Chiarotti, and N. Marzari. *On Green's function embedding from sum-over-poles representations.* Phys. Rev. B 110, 045149 (2024).
[4] T. Chiarotti, A. Ferretti, and N. Marzari. *Energies and spectra of solids from the algorithmic inversion of localized GW.* Phys. Rev. Research 6, L032023 (2024).
[5] T. Chiarotti, N. Marzari, and A. Ferretti. *A unified Green's function approach for spectral and thermodynamic properties from algorithmic inversion of dynamical potentials.* Phys. Rev. Research 4, 013242 (2022).
[6] M. Quinzi, T. Chiarotti, M. Gibertini, and A. Ferretti. *Broken symmetry solutions in one-dimensional lattice models via many-body perturbation theory.* Phys. Rev. B, in press (2025).

[P1.48] Modeling Spectroscopic Properties of Biomolecules

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Spectroscopic techniques including infrared (IR) spectroscopy are widely used methods particularly useful in probing the structural organization of (bio)molecular systems, including proteins and nucleic acids. In fact, several IR bands are highly sensitive to the changes in the structural organization of biomolecular assemblies. One of the most used signals is that arising from C=O stretching vibrations as it proved to display relevant changes depending on, e.g., the secondary structure in peptides and proteins or distinct structural motifs in nucleic acids. Nevertheless, the direct mapping between IR spectral bands and specific structural features is not straightforward, in particular for systems with a rugged conformational landscape. Here, we use a tandem quantum/classical computational approach based on the perturbed matrix method (PMM-MD) formalism [1] for the calculation of IR spectra. This approach has been already successfully applied to the calculation of IR spectra in polypeptides, both in the amide I region [2] and for specific side chains bands [3,4]. Here, it is extended to compute IR bands in DNA nucleobases. More specifically, we compute the IR spectrum arising from C=O stretching modes of all carboxyl containing bases, i.e., thymine, guanine and cytosine, in both water and deuterated water. We use as a first benchmark the isolated bases in solution, both with and without the ribose and phosphate moieties. Then, we move to more extended systems and compute the spectra of single-stranded deca-homonucleotides. Finally, we consider an aptamer whose sequence embodies the combination of all nucleic acid building blocks. The comparison of the calculated spectra with the corresponding experimental spectra shows an overall good agreement. Most importantly, our approach shows to be able to reproduce the experimentally observed variations in the spectral signals due to conformational diversity, including stacking and hydrogen bonding interactions among the bases.

References

[1] L. Zanetti-Polzi, S. Del Galdo, I. Daidone, M. D'Abramo, V. Barone, M. Aschi, and A. Amadei. *Extending the perturbed matrix method beyond the dipolar approximation: comparison of different levels of theory.* PCCP 20, 24369-24378 (2018).

[2] C. M. Davis, L. Zanetti-Polzi, M. Gruebele, A. Amadei, R. B. Dyer, and I. Daidone. *A quantitative connection of experimental and simulated folding landscapes by vibrational spectroscopy.* Chem. Sci. 9, 9002-9011 (2018).

[3] S. M. Vieira Pinto, N. Tasinato, V. Barone, A. Amadei, L. Zanetti-Polzi, and I. Daidone. *Modeling amino-acid side chain infrared spectra: the case of carboxylic residues.* PCCP 22, 3008-3016 (2020).

[4] S. M. Vieira Pinto, N. Tasinato, V. Barone, L. Zanetti-Polzi, and I. Daidone. *A computational insight into the relationship between side chain IR line shapes and local environment in fibril-like structures.* JCP 154, 084105 (2021).

Abstracts | Poster Presentations Day 2 (June 06, 2025)

[P2.01] Acoustic Biosensors for the detection of disease-related biomarkers

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Neurodegenerative diseases and infectious viral pathogens represent major global health challenges, requiring advanced diagnostic tools for early detection and monitoring. Biosensors based on acoustic wave technologies have emerged as promising platforms for the selective and sensitive detection of biomolecular targets in biological fluids [1-2]. A critical aspect of biosensor development is the functionalization of sensor surfaces to ensure efficient molecular recognition, minimal non-specific adsorption, and optimal signal transduction.

This study explores different chemical functionalization strategies for acoustic biosensors, focusing on the immobilization of bioreceptors for the detection of disease-related biomarkers. Two case studies are considered: (i) the detection of Alzheimer's disease (AD)-related proteins, specifically amyloid-β (Aβ42 and Aβ40), and (ii) the identification of the West Nile Virus (WNV) infection through the detection of the NS1 glycoprotein. In both applications, sensor surfaces were modified with self-assembled monolayers (SAMs) composed of thiol-functionalized molecules, including 12-mercaptododecanoic acid (MDA) and polyethylene glycol (PEG) derivatives of varying molecular weights. These adlayers provided carboxyl-functionalized surfaces for covalent attachment of antibodies or aptamers, ensuring specific biomolecular recognition.

For AD biomarker detection, antibody-based and aptamer-based bioreceptors were immobilized, with results showing effective surface coverage and molecular binding as evaluated by frequency and dissipation shifts in Quartz Crystal Microbalance with Dissipation monitoring (QCM-D) measurements. The incorporation of PEG molecules demonstrated antifouling properties, reducing non-specific adsorption while maintaining target recognition efficiency. Similarly, for WNV detection, an antibody specific for the NS1 glycoprotein was immobilized onto chemically activated sensor surfaces. A comparative analysis of different adlayer compositions, including different-molecular-weight PEGs, revealed a correlation between molecular density and antifouling properties, providing an optimal balance between surface passivation and antibody immobilization efficiency.

These findings highlight the crucial role of surface chemistry in optimizing biosensor performance, particularly in terms of specificity, stability, and resistance to non-specific binding. The insights gained from these studies contribute to the development of next-generation acoustic biosensors for point-of-care diagnostics, enabling rapid and reliable biomarker detection for neurodegenerative diseases and viral infections.

References

[1] M. Agostini, et al. Advanced Functional Materials 32(44), (2022).
[2] M. Gagliardi, et al. *Surface acoustic wave-based lab-on-a-chip for the fast detection of Legionella pneumophila in water.* Sensors and Actuators B: Chemical 379, (2023).

Projects

Next Generation EU, Mission 4 Component 2 Inv. 1.5 (Tuscany Health Ecosystem, Spoke 4).
Next Generation EU, Mission 4 Component 2 Inv. 1.3 (One Health Basic and Translational Research Actions Addressing Unmet Needs on Emerging Infectious Diseases (INF-ACT), Spoke 5).

[P2.02] Maternal Immune Activation Induces Persistent Functional Alterations in Astrocytes of the Somatosensory Cortex, a 2-photon excitation laser scanning microscopy study

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Inflammation during embryonic development or in preterm infants is linked to neurodevelopmental disorders such as autism spectrum disorder (ASD) or attention-deficit/hyperactivity disorder (ADHD). These lifelong conditions are increasing dramatically and represent a health priority worldwide. Understanding all molecular and cellular events involved in these disorders is crucial to develop new specific therapies. During development, astrocytes play a key role in synaptic and neuronal maturation.

Here we tested whether maternal immune activation affects astrocytic functions later in young adults. We used multiphoton laser scanning microscopy to perform calcium imaging experiments in astrocytes of somatosensory cortical slices from 8 weeks old mice, soon after development has completed. Astrocytic expression of GCaMP6f and tdTomato was achieved with injections of AAV vectors in somatosensory cortex. As expected from previous studies of our group and others, astrocytes showed spontaneous calcium events mainly as microdomains, i.e., small events in the ultrathin processes that represent most of the astrocyte volume, with respect to soma and major branches in which events were rarer. In small processes of layer II/III astrocytes, calcium events in slices from LPS mice were significantly more frequent than in controls. Furthermore, the average area of calcium events was significantly larger in LPS mice than controls. In particular, distribution of calcium event area revealed that LPS astrocytes presented an increased portion of events with larger area and reduced percentage of more localized events. Amplitude was instead reduced in LPS mice while duration was unaltered. Our data reveal that two months after immune activation, young adult mice have altered calcium activity in small processes of somatosensory cortex astrocytes, a region involved in ASD and AHDH. Increased frequency and reduced localization of calcium events in astrocytes likely affect synaptic modulation in that region. Finally, astrocyte contributes to neurodevelopment by releasing several factors including neurosteroids (NS), important modulatory and neuroprotective molecules. We are thus analyzing brain NS content and steroidogenic enzymes expression in control and MIA offspring at different time points during development by LC-MS and immunohistochemistry. Altogether our data help to elucidate the molecular and cellular events involved in neurodevelopmental disorders linked to prenatal or neonatal immune activation, possibly revealing new targets for future therapies.

[P2.03] Liquisens: A Dual-Mode SAW Sensor on 64° Y-Cut Lithium Niobate for Advanced Real-Time Sensing and Mixing in Liquid Environments

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This study focuses on the design, fabrication, and characterization of Liquisens: an innovative dual-mode surface acoustic wave (SAW) sensor on a 64° Y-cut lithium niobate (LN) substrate. The ability to generate both Rayleigh SAW (R-SAW) and shear horizontal SAW (SH-SAW) on the same 64° Y-cut LN piezoelectric substrate enables the exploitation of its high electromechanical coupling for the development of a highly efficient sensing platform.

The starting point of this work is based on our previous study, where we presented an innovative dual-mode SAW configuration utilizing a 64° Y-cut LN substrate. The conventional setup, employing interdigital transducers (IDTs) oriented along the crystal X-axis, is known for generating SH-SAW modes with in-plane polarization. Conversely, by utilizing IDTs oriented perpendicular to the X-axis, we effectively introduced the excitation of a Rayleigh-like SAW (R-SAW), a novel achievement in our research. We conducted a comprehensive characterization of the innovative R-SAW mode, from electromechanical coupling to liquid wave interaction.

Building upon these findings, we developed Liquisens platform, composed of multiple SH-SAW sensors, each equipped with individual interdigital transducers (IDTs). These IDTs were analyzed in reflection using S11 parameters, enabling continuous monitoring of resonance frequencies. This approach allows for real-time sensing in liquid environments. Additionally, the platform includes a central IDT capable of generating R-SAW for mixing implementation through acoustic streaming. This dual-functionality configuration enables simultaneous sensing and mixing, supporting multiplexed detection in diverse environments. Furthermore, the piezoelectric chip is integrated with a microfluidic channel, optimizing sample analysis and manipulation.

Following fabrication and characterization, covering both electromechanical properties and mixing efficiency, the Liquisens sensor was tested for its ability to measure the physicochemical properties, specifically viscosity and density, of water-alcohol mixtures. The sensor's mass-loading response was then evaluated by monitoring the adhesion of bovine serum albumin proteins onto the gold-sensitive surface.

Finally, to explore potential agrifood applications, the sensor was evaluated in a case study for detecting polyphenol mixtures within synthetic wine matrices. The sensor surface was functionalized with a specific peptide designed for selective binding of tannins, key polyphenolic compounds influencing wine quality and characteristics. Binding interactions were systematically analyzed, and a calibration curve was established by measuring sensor responses across a range of polyphenol concentrations. This approach enabled the evaluation of the sensor's sensitivity, specificity, and dynamic range, demonstrating its potential for accurate and real-time monitoring of polyphenolic content in complex liquid matrices such as wine.

These results demonstrate the versatility and potential of the Liquisens platform for advanced real-time sensing applications in different liquid environments, paving the way for its integration into real-world analytical and industrial processes.

[P2.04] Green Nanotechnology-Enhanced Photodynamic Therapy for Cancer Treatment

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Photodynamic therapy (PDT) has emerged as a promising, minimally invasive approach for cancer treatment, utilizing photosensitizers activated by light to generate cytotoxic reactive oxygen species (ROS) [1]. Hypericin (Hyp), a naturally derived photosensitizer, exhibits strong photodynamic effects and selective tumor-targeting properties [2]. However, its hydrophobic nature and tendency to aggregate limit its clinical applications. To enhance hypericin's bioavailability and efficacy, green chemistry-based nanoparticle formulations have been developed as eco-friendly and biocompatible delivery systems [3]. We recently developed a novel approach based on green chemistry to obtain gold and silver nanoparticles through the reducing action of Hyp (Fig. 1A), avoiding the use of toxic reagents. Hyp reduces gold and silver precursors, producing nanoparticles (NPs) ranging from 10 to 20 nm in size. Hyp remains attached to the NPs, allowing cancer cell treatment via PDT, in which green light irradiation triggers Hyp-dependent production of ROS (Fig. 1D), decreasing cells viability (Fig. 1E). Preliminary data showed that Hyp concentration used for PDT is much lower than the calculated IC_{50} (1.5 µM) and has no toxic effects in the absence of irradiation. These NPs improve hypericin's solubility, stability, and tumor accumulation while reducing systemic toxicity. By integrating green nanotechnology with PDT, this approach offers a sustainable and effective strategy for cancer therapy, paving the way for innovative advancements in oncological treatments.

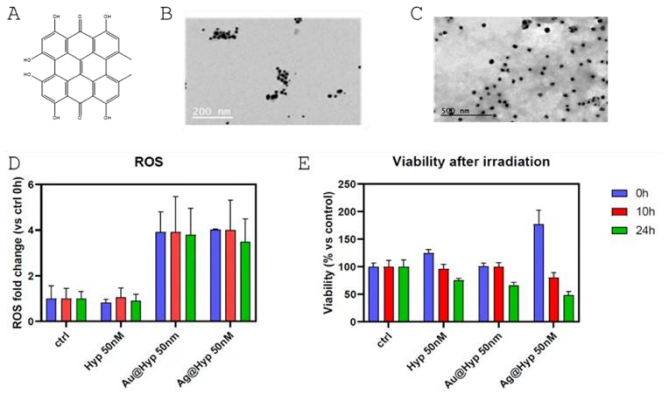

Fig. 1: ROS production in GL261 cell line. A) Hyp structure. B) Gold (Au@Hyp) and C) Silver (Ag@Hyp) NPs produced with Hyp. D) ROS production after treatment of GL261 cells with Hyp, Au@Hyp or Ag@Hyp at a final concentration of 50Nm and then irradiated for 2 minutes. ROS were measured after 0, 10 and 24h. E) Viability of cells after irradiation (same conditions used for ROS measurements).

References

[1] W. Jiang, M. Liang, Q. Lei, G. Li, and S. Wu. *The Current Status of Photodynamic Therapy in Cancer Treatment. Cancers 15* (3), 585 2023.

[2] X. Dong, Y. Zeng, Z. Zhang, J. Fu, L. You, Y. He, Y. Hao, Z. Gu, Z. Yu, C. Qu, X. Yin, J. Ni, and L. J. Cruz. *Hypericin-Mediated Photodynamic Therapy for the Treatment of Cancer: A Review.* Journal of Pharmacy and Pharmacology 73, 425–436 (2021).

[3] N. Choudhary, T. E. Collignon, D. Tewari, and A. Bishayee. *Hypericin and Its Anticancer Effects: From Mechanism of Action to Potential Therapeutic Application*. *Phytomedicine 105*, 154356 (2022).

[P2.05] Novel Graphene-based biosensor for opto-electronic detection of proteins at zepto-molar concentration

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We demonstrate a novel *label-free* two-terminal opto-electronic graphene biosensor, capable of detecting the immunoglobulin M at the remarkably low concentration of 100 zeptomolar (10^{-19} M). [1] Our data clearly show that the binding of approximately 6 ± 2 antigens to an equal number of capture sites affects the surface potential on a gold gate area hosting at least 10^7 antibodies. Such an extended surface potential change modulates the graphene channel carrier concentration and Fermi level. These changes are transduced into shifts of the graphene phonon frequencies, which are readily detected *in-situ* by Raman spectroscopy and correlated via a simple model to the shift of the charge neutrality point of graphene. The data are also corroborated by Kelvin probe force microscopy experiments [2-3].

The integration of graphene with optical probing establishes a ground-breaking approach to *in-situ* biomarker detection and sets the stage for a future generation of portable opto-electronic high-performance diagnostic tools for single-markers detection. Our two-terminal electric scheme, which is considerably simpler than the conventional transistor-like one [4], minimizes potential sources of noise, and potentially enhances sensor reliability. Moreover, the use of an electrolyte-soaked paper strip for the coupling between the biofunctionalized gate electrode and the graphene channel provides an effective means of maintaining a stable liquid environment, aligning with the growing interest in developing self-contained, pump-free microfluidic platforms driven by capillary forces. Such a sensor design choice, coupled with the unique optoelectronic properties of graphene and the powerful probing capabilities of Raman spectroscopy, has enabled us to achieve single molecule regime sensitivity in label-free biomarker detection. In perspective, the increasing availability of portable Raman spectrometers opens to the development of a portable graphene-based platform.

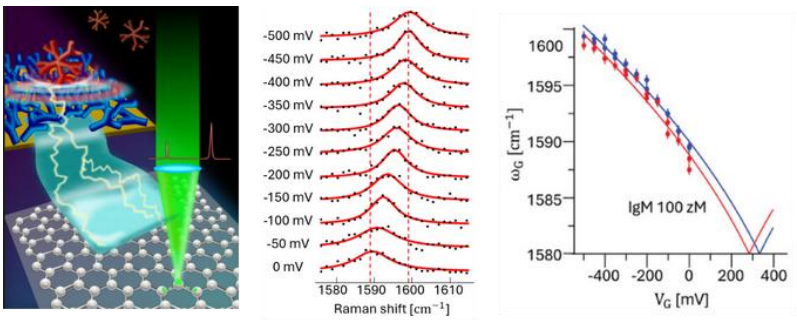

Fig. 1: An opto-electronic graphene-based biosensor detects immunoglobulin M (IgM) at 100 zeptomolar (10-19 M) concentration. It features a biofunctionalized gold electrode capacitively coupled to a graphene electrode via a water-soaked paper strip. Surface potential changes induced by few affinity events are transduced as shifts of the graphene phonon frequencies and detected by Raman spectroscopy.

References

[1] M. Piscitelli, et al. *Graphene-based opto-electronic detection of few proteins.* Small Methods, 2402026 (2025).
[2] C. Di Franco, et al. Advanced Materials Interfaces, 2201829 (2023).
[3] C. Di Franco, et al. J. Mat. Chem. C 12, 73 (2024).
[4] E. Macchia, et al. Chemical Reviews 122, 4636 (2022).

[P2.06] Single-molecule and multiscale fluorescence imaging to investigate pd-l1 dynamics and its association with lipid rafts in non-small cell lung cancer cells

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The membrane protein Programmed Death Ligand 1 (PD-L1) plays a pivotal role in various human tumors and has recently emerged as a key target for cancer therapy, with clinical studies demonstrating the effectiveness of immunotherapeutic treatment [1]. While the immunosuppressive function of the PD-1/PD-L1 immune checkpoint is well characterized, the molecular mechanisms underlying its regulation at the nanoscale remain poorly understood [2] and are likely influenced by its spatial organization and diffusional properties.

In this study, we employed a combination of super-resolution and single-molecule fluorescence imaging techniques to investigate the nanoscale organization and dynamic behavior of PD-L1 in the plasma membrane of non-small cell lung cancer (NSCLC) cells. Using Single-Molecule Localization Microscopy (SMLM), we revealed that PD-L1 is predominantly organized in nanoscale clusters (~30-40 nm in radius) within cholesterol-enriched membrane raft domains. Functional colocalization studies with key lipid raft markers confirmed this preferential association.

Furthermore, Fluorescence Correlation Spectroscopy (FCS) and spot variation-STED-FCS in live cells allowed us to probe PD-L1 diffusion at the single-molecule level, uncovering a confined diffusion behavior characteristic of raft-associated proteins. This suggests that PD-L1 mobility and molecular interactions are tightly regulated by the biophysical properties of membrane microdomains.

The implications of PD-L1 raft engagement extend beyond its canonical immune function. Preliminary evidence suggests that this association may modulate PD-L1/PD-1 immune checkpoint activity, providing new insights into immune evasion mechanisms and potential therapeutic strategies in immuno-oncology. Additionally, the existence of a non-clustered, more freely diffusing PD-L1 population hints at potential alternative functions unrelated to immune suppression.

To further validate our findings, we are currently performing PhotoActivated Localization Microscopy (PALM) using a photoswitchable PD-L1 construct. This approach enables a direct comparison between single-molecule localization data obtained with antibody-based labeling and genetically encoded fluorescence, providing complementary insights into PD-L1 spatial distribution and dynamics. Ongoing experiments aim to further elucidate these aspects.

By integrating multiscale fluorescence imaging with single-molecule biophysics approaches, this study provides a deeper understanding of PD-L1's spatial organization and dynamic behavior, shedding light on its potential role in NSCLC pathophysiology and targeted therapeutic interventions.

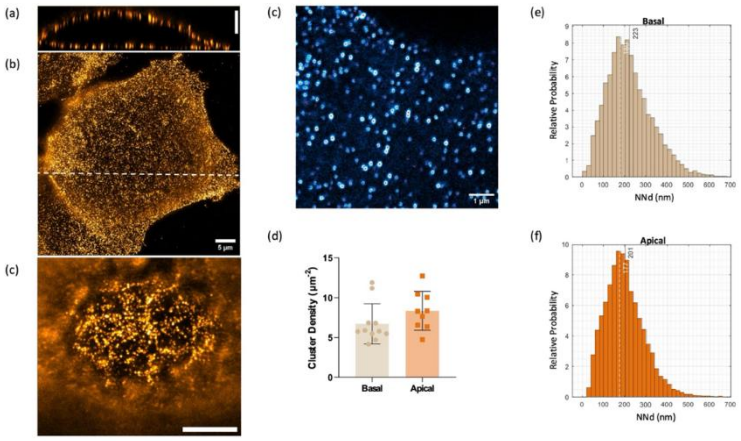

Fig.1: SPLIT-STED images of a HCC827 cell. a) orthogonal b) basal and c) apical section. Scale bar: 5 µm. c) Crop of a SPLIT-STED image of a basal membrane edge analyzed by ThunderSTORM. The identified cluster are marked with a red cross. Scale bar 1 µm.

d) Cluster density obtained as the ratio between number of clusters identified over area. The two distributions are not statistically different: p=0.1 Mann Whitney test. e) Nearest neighbours' distance for the basal and f) apical sections.

References

[1] A. Kythreotou, A. Siddique, F. A. Mauri, M. Bower, and D. J. Pinato. *PD-L1.* J Clin Pathol 71, 189-194 (2018).

[2] K. Esfahani, et al. Current Oncology 27, S87-S97 (2020).

[3] L. Roudaia, N. Buhlaiga, S. V. Del Rincon, N. Papneja, and W. H. Miller. *A review of cancer immunotherapy: from the past, to the present, to the future.* Current Oncology 27, S87-S97 (2020).

[P2.07] Nanomedicine for neurodevelopmental disorders: nanomaterials to study and to treat Angelman Syndrome

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Recent decades have seen a dramatic increase in neurodevelopmental disorders (NDD). Ubiquitin ligase E3A (UBE3A) plays a key role in the brain and changes in its expression levels lead to NDD: its loss causes Angelman syndrome (AS) while its increase autisms. AS presents neuronal connectivity and plasticity deficits, however, UBE3A function in brain pathogenesis is still unclear.
A promising therapy for AS is on the way, based on antisense oligonucleotides (ASO) to restore UBE3A expression. ASO, short single-stranded nucleic acid molecules with high therapeutic potential, cannot cross the blood brain barrier (BBB) and require invasive administration methods (intrathecal inj.) to reach the brain.
Monitoring NDD progression and the effects of therapies is complex and requires invasive procedures or behavioural observations (highly prone to subjective bias). Today there is a high need of quantitative biomarkers of brain function, in NDD and in particular in AS. Small extracellular vesicles (< 200 nm) of neural origin (NEVs) can cross the BBB and are a potential window into the brain status.
Our goal is to exploit novel nanotools for improving the knowledge and the therapeutic development in AS:
1) We develop and validate nano/micro-structured substrates, combining directional nano/micro-topographies (GRatings) and mechanical cues, by solvent casting. These substrates are tested in vitro with Wild-Type and AS neuronal cells as advanced biomimetic platforms, to study neuronal mechanosensing and migration processes. Deficits in contact guidance [1] and migration in AS neurons emerge on GRs.
2) We develop nanoparticles (NPs) for the brain delivery of ASO via the non-invasive intranasal route. We formulate NPs made of biocompatible polymers, by cross-linking strategies. These chitosan and Poly(Lactic-co-Glycolic) Acid NPs show optimal physico-chemical properties, biocompatibility with neuronal and nasal cells [2], and muco-adhesion features in vitro.
3) We develop a clinical assay based on the selective enrichment of NEVs, from WT/ AS neuronal cells and plasma samples, with the aim to identify molecular biomarkers deregulated in AS. The assay allows the collection of NEVs via size exclusion chromatography and immunocapture, and their proteomic analysis. Results show differences in the levels of proteins involved in cell adhesion and migration in AS samples.
Nanotools such as GRs, NPs and NEVs assay can positively impact AS NDD, allowing us to identify new potential therapeutic targets, to improve ASO therapy, and to monitor the therapies or follow-up of AS patients.

References
[1] I. Tonazzini, et al. Mol Autism 10, 41 (2019).
[2] M. Gagliardi, et al. Int J Mol Sci 24, 6590 (2023).

Projects
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MUR PRIN-Next Gen EU 2022 grant ENGInerve (PE11).

[P2.08] Assessing Wine Polyphenols via Quartz Crystal Microbalance with Dissipation Monitoring and Fluorescence Lifetime Imaging Microscopy

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Polyphenols play a crucial role in winemaking, influencing essential characteristics such as quality, color, astringency, bitterness, and chemical stability [1]. However, traditional methods for polyphenol quantification are often costly and time-consuming, necessitating alternative approaches [2].

This study explored the use of *Quartz Crystal Microbalance with Dissipation Monitoring* (QCM-D) for polyphenol analysis in red wines, employing *Gelatin Type A* (Gel-A) and *Mouse Proline-Rich Protein 5* (MP5) as molecular probes. They were still tested in the analysis of different tannin families in aqueous solutions and in artificial wines, demonstrating their effectiveness [3, 4]. Both probes were successfully immobilized onto the sensor surface, achieving molecular densities of 2.1×10^{14} and 5.1×10^{12} molecules/cm², respectively. *Atomic Force Microscopy* (AFM) characterization confirmed the formation of a network-like structure for both probes.

Gel-A and MP5 demonstrated effective polyphenol detection, as indicated by shifts in resonance frequency and dissipation. Notably, MP5 exhibited a linear dissipation response correlated with total polyphenol and hydroxybenzoic acid concentrations, highlighting its potential for real-time monitoring in winemaking.

Additionally, *Fluorescence Lifetime Imaging Microscopy* (FLIM) combined with phasor analysis (FLIM-ϕ) was explored as a novel approach to characterize the polyphenol profile of wines. This method generates a fingerprint-like diagram, allowing for rapid wine discrimination based on aging, grape variety, and origin.

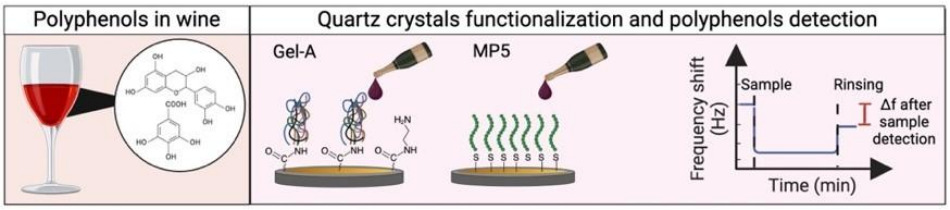

Fig. 1: Chemical functionalization and detection of polyphenols in wines by QCM-D.

References

[1] R. Gutiérrez-Escobar, M. J. Aliaño-González, and E. Cantos-Villar. *Wine Polyphenol Content and Its Influence on Wine Quality and Properties: A Review.* Molecules 3-26, 718 (2021).

[2] M.C. Vlasiou. *Cheese and Milk Adulteration: Detection with Spectroscopic Techniques and HPLC: Advantages and Disadvantages.* Dairy 3-4, 509 (2023).

[3] M. Gagliardi, G. Tori, M. Agostini, F. Lunardelli, F. Mencarelli, C. Sanmartin, and M. Cecchini. *Detection of Oenological Polyphenols via QCM-D Measurements.* Nanomaterials 1-12, 166 (2022).

[4] M. Gagliardi, G. Tori, C. Sanmartin, and M. Cecchini. *The effect of probe density coverage on the detection of oenological tannins in quartz crystal microbalance with dissipation monitoring (QCM-D) experiments.* Journal of the Science of Food and Agriculture 105(3), 1476-1483 (2025).

[P2.09] Development of Coarse Grained Force fields of Polymeric Materials for Sustainable Food Packaging

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Food packaging is essential to ensure an adequate stability of the product throughout its entire shelf life. Currently, multiwall polymers are the preferred choice due to their excellent mechanical and barrier properties against oxygen and moisture. Unfortunately, their recycling is difficult and costly, often becoming plastics of single use.[1] Understanding of the structural and dynamic properties of polymers is crucial to develop more sustainable alternatives. However, the computational modelling of these materials poses a great challenge due to the fact that their dynamics span over several time scales.[2] As a result, a multiscale approach becomes mandatory to gain access to the slower degrees of freedom. In this regard, coarse grained (CG) models have drawn considerable attention in recent years.[3] CG models neglect the fastest degrees of freedom flattening the rugged potential energy surface (PES) and thus, allowing higher time steps. In this work, a set of different coarse grained force fields (CG-FFs) are developed with the iterative Boltzmann inversion (IBI) for polyethylene terephthalate (PET) and its bio-based counterpart polyethylene furandicarboxylate (PEF). A systematic study of the effect of the choice of CG mapping scheme is carried out on the structural properties of these polymers.

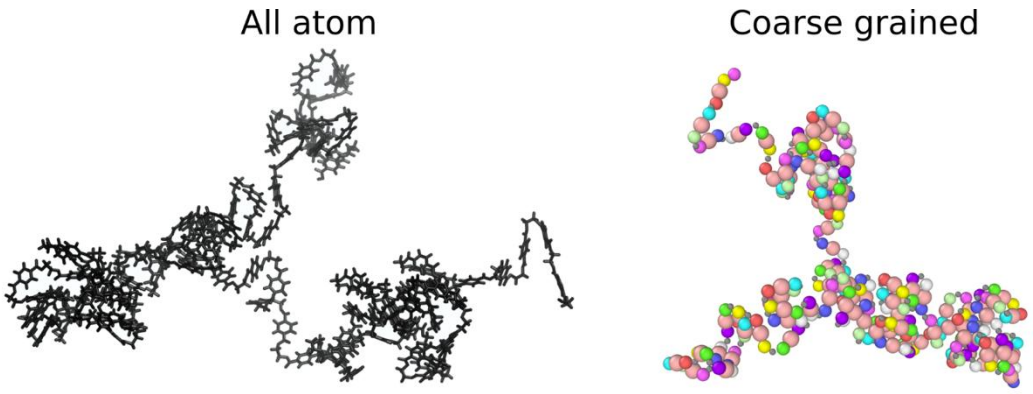

Fig. 1: Model of a polymer chain in all atom (left) and coarse grained (right) representation.

References

[1] V. Guillard, S. Gauce, C. Fornaciari, H. Angellier-Coussy, P. Buche, and N. Gontard. *The Next Generation of Sustainable Food Packaging to Preserve Our Environment in a Circular Economy Context.* Front. Nutr. 5, 121 (2018).

[2] R. B. Bird, R. C. Armstrong, and O. Hassager. *Dynamics of Polymeric Liquids. Volume 1: Fluid Mechanics*, 2nd ed. (1987).

[3] K. Kempfer, J. Devémy, A. Dequidt, M. Couty, and P. Malfreyt. *Development of Coarse-Grained Models for Polymers by Trajectory Matching.* ACS Omega 4-3, 5955 (2019).

[P2.10] Optical Control of Energy Transfer in Strongly Coupled Organic Microcavities

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In recent decades, extensive research has been dedicated to exploring and advancing organic microcavities that facilitate strong light-matter coupling. Within these structures, the interaction between photons and excitons surpasses the intrinsic damping mechanisms of the system, resulting in the formation of hybrid radiation-matter states, known as cavity polaritons [1]. One of the most promising applications of organic polaritons stems from their inherently delocalized nature, which can be harnessed to facilitate long-range energy transfer. Both theoretical and experimental investigations have demonstrated that energy transfer mediated by polaritons can extend over distances of 1–2 micrometers. However, such systems generally remain static, as they are determined by the specific cavity configuration. Nevertheless, the ability to modify polariton energy via external optical stimuli [2] could unlock new and exciting possibilities for optimizing energy flow in photonic systems. In this work, dynamic control is shown by utilizing photochromic molecules as active component of a Fabry-Perot microcavity. The concentration of the photochromic donor component was modulated using optical UV and visible signals, enabling direct control over the light-matter coupling constant and, consequently, the polariton formation and energy transfer dynamics. By analyzing the photoluminescence spectra of the system, the efficiency of the energy transfer process was evaluated, revealing an approximately six-fold increase in the relative contribution of acceptor species to the total emission when the multilayer was confined within the resonant cavity compared to its placement outside the microcavity [3]. These findings provide a foundation for the development of dynamic systems in which energy transport is governed by light stimuli, with potential applications in light harvesting, light-emitting devices, and photovoltaic technologies.

References

[1] V. M. Agranovich and G. F. Bassani. *Thin Films and Nanostructures: Electronic Excitations in Organic Based Nanostructures.* Elsevier Academic Press, London, 31 (2003).

[2] P. A. Thomas, K. S. Menghrajani, and W. L. Barnes. *All-optical control of phase singularities using strong light-matter coupling.* Nature Communications 13, 1809 (2021).

[3] A. Cargioli, M. Lednev, L. Lavista, A. Camposeo, A. Sassella, D. Pisignano, A. Tredicucci, F. J. Garcia-Vidal, J. Feist, and L. Persano. *Active control of polariton-enabled long-range energy transfer.* Nanophotonics 13-14, 2541-2551 (2024).

Project

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[P2.11] Reconfigurable Beamforming Metasurfaces for Infrared Beam Steering

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Metasurfaces are emerging as key components for compact and efficient beam-steering and optical control applications. Our research focuses on the design and optimization of tunable metasurfaces including chalcogenide glasses (such as GeSeTe, GeSeSbTe, Se_2S_3, and Se_2Sb_3) as active materials. These materials can dynamically modulate their refractive index in response to external stimuli, including electric fields, temperature changes, or pulsed lasers. By integrating chalcogenide glasses with silicon resonators, we achieve low-loss transmissive pixels capable of a full 0 to π phase shift. Moreover, these glasses exhibit non-volatile switching between amorphous and crystalline states, eliminating the need for additional electronic components, such as thin-film transistors, commonly required in liquid crystal-based devices [1,2].

To optimize the design of these phase-controlling pixels, including all the device elements such as layers including ridges of ITO electrodes, we employed a tailored optimization algorithm with suitable loss functions, ensuring minimal optical losses and high efficiency. We then validated the metasurface's performance by demonstrating its ability to steer a beam at a telecommunications-relevant wavelength of 1550 nm. Our findings highlight the potential of chalcogenide-integrated metasurfaces for next-generation reconfigurable optics and beam-steering applications.

a) b) c)

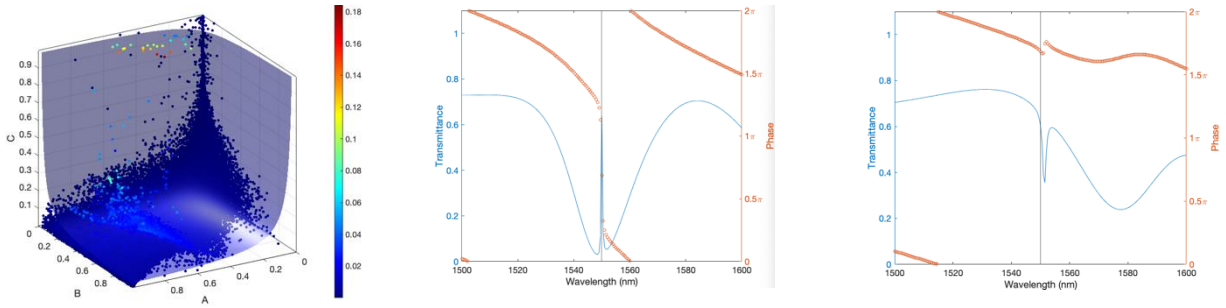

Fig. 1: a) three-dimensional plot of the optimized set of parameters returning the Figure of Merit given by the $fom = \sqrt{A \cdot B \cdot C^2}$ where $C=\left(\frac{\Delta\phi}{\pi}\right)$ and $\Delta\phi = \frac{angle(\frac{t_A}{t_C})^2}{\pi^2}$. b,c) transmittance and phase calculated for a specific set of parameters for amorphous and crystalline GeSeTe, respectively.

References

[1] S. Mansha, et al. *High resolution multispectral spatial light modulators based on tunable Fabry-Perot nanocavities.* Light: Science & Applications 11, 141 (2022).

[2] G. E. Lio and A Ferraro. *LIDAR and Beam Steering Tailored by Neuromorphic Metasurfaces Dipped in a Tunable Surrounding Medium*. Photonics 8, 65 (2021).

[P2.12] Probing THz-light driven phenomena in quantum materials at the nanoscale

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Scattering-type scanning near-field optical microscopy (s-SNOM) in the terahertz (THz) range is a powerful tool for characterizing the nanoscale properties of quantum materials, including topological insulators [1], van der Waals heterostructures (vdWHs) [2] and nanophotonic resonators [3,4]. These materials exhibit unique optical and electronic characteristics at the nanometer scale, such as hyperbolic surface phonon polaritons (HSPhPs) [5] and other quasiparticles surpassing the diffraction limit [6]. A deeper understanding of these features enables precise engineering of the material nanoscale response, paving the way for the development of tunable platforms for advanced photonic and opto-electronic applications [2].

Herein, we will provide an overview of our state-of-the-art THz near-field nanoscopy and spectroscopy detectorless approaches for the characterization of quantum materials and nanodevices, highlighting recent advancements and challenges in the field [3-5,7-13]. Additionally, new perspectives on the potential applications of engineered nanostructures will be discussed, emphasizing their role in the future of nanophotonics and quantum technologies.

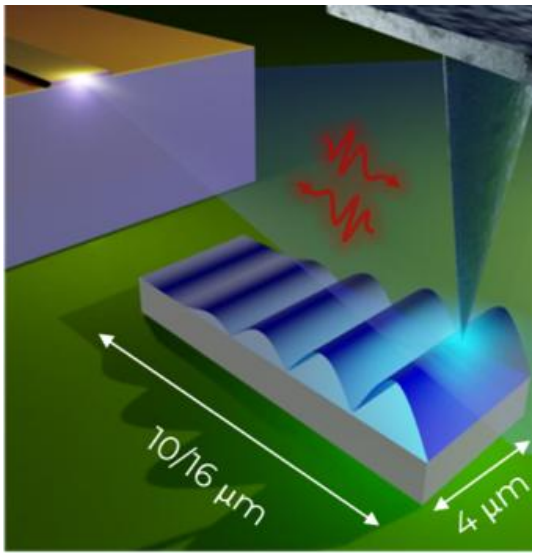

Fig. 1: Schematics of THz Dirac plasmon polaritons (DPPs) of a Bi_2Se_3 antenna resonator launched by the s-SNOM tip under excitation with a THz quantum cascade laser (QCL) (adapted from [4]).

References

[1] S. Chen, et al. Nat. Commun. 13(1), 1–9 (2022).
[2] X. Guo, et al. Appl. Phys. Rev. 11(2), 21306 (2024).
[3] C. Schiattarella, et al. Sci. Rep. 14(1), 1–11 (2024).
[4] V. Pistore, et al. Small 2308116 (2023).
[5] E. A. A. Pogna, et al. Nat. Commun. 12(1), 1–11 (2021).
[6] D. N. Basov, et al. Light Sci. Appl. 9, 189 (2020).
[8] E. A. A. Pogna, et al. APL Photonics 6, 061302 (2021).
[9] K. S. Reichel, et al. Nanophotonics 10(5), 1495-1503 (2021).
[10] V. Pistore, et al. Adv. Sci. 9(28), 2200410 (2022).
[11] V. Pistore, et al. Adv. Opt. Mat. 12(4), 2301673 (2024).
[12] V. Pistore, et al. Appl. Phys. Lett. 124, 221105 (2024).
[13] L. Viti, et al. *Tracing terahertz plasmon polaritons with a tunable-by-design dispersion in topological insulator metaelements.* Accepted for publication in Light Sci. Appl. (in press).

[P2.13] Gate Tunable ON-OFF Hybrid Superconducting Electronics

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Hybrid superconducting-semiconducting electronics is the emerging star in cryogenic fast and ultra-low power solid-state quantum electronics [1]. The central component of the hybrid superconducting-semiconducting technology is the hybrid Josephson Junction (JJ), which consists of a semiconductor positioned between two superconducting leads. The control of the supercurrent, or non-dissipative current, in a hybrid JJ can be achieved by designing the device architecture to include a gate electrode, allowing for the realization of a Josephson Field Effect Transistor (JoFET). Figs. 1a and 1b illustrate the two fundamental blocks alongside their respective electrical symbols. Controlling the charge density of the semiconductor with the gate voltage enables the tuning of both the superconducting and normal transport properties of the JoFET. As the charge density decreases, the supercurrent (I_S) also decreases, while the resistance in the normal dissipative state (R_N) increases (Fig. 1b).

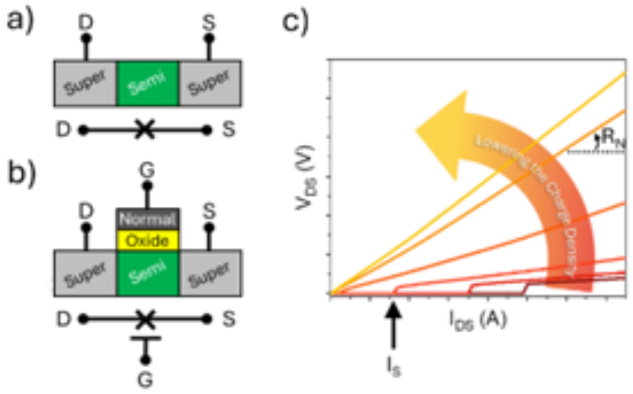

Fig. 1: a,b) The structure and schematic symbols of a JJ (a) and a JoFET (b). c) The V_{DS} versus I_{DS} characteristics of a JoFET resulting from the reduction of semiconductor charge density when applying gate voltage.

For a specific class of applications, users are primarily interested in tuning the supercurrent. However, for other applications, completely suppressing the supercurrent and achieving significant variations in the transport properties of the JoFET is essential for satisfactory circuit performance. One example of this is the routing of supercurrent, where multiple JoFETs are integrated on the same chip and connected via superconducting traces to direct non-dissipative currents [2]. Fig. 2a illustrates a superconducting demultiplexer (DEMUX) with one input and two outputs that incorporates two JoFETs. The JoFET on the top is in the superconducting ON state, while the JoFET on the bottom is gated into the dissipative OFF state. This configuration defines the ON and OFF branches, with flowing currents labeled as I_{ON} and I_{OFF}, respectively. Fig. 2b shows the ratio of I_{OFF} to I_{ON} as a function of R_L/R_N, where R_L represents the load impedance. For R_N/R_L greater than 100, the ratio I_{OFF}/I_{ON} approaches 0, which indicates that all the current flows as supercurrent in the ON branch. As R_N/R_L decreases, the ratio I_{OFF}/I_{ON} approaches 0.5, demonstrating that regardless of the state of the JoFETs, the current is evenly divided between the two branches. This example clearly highlights the importance of gate tunability on both the superconducting and normal transport properties of the JoFET.

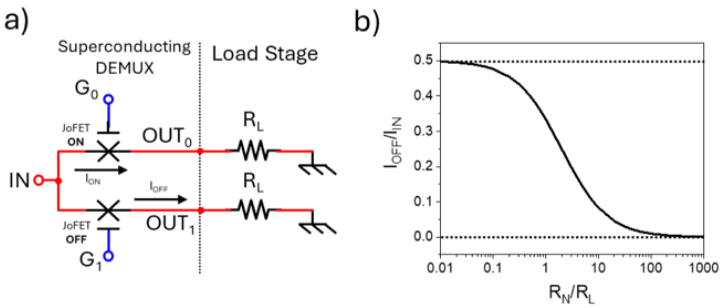

Fig. 2: a) Schematic circuit of a superconducting DEMUX with the load stage. b) Ratio between the current flowing in the OFF and ON branch as a function of R_N/R_L.

References

[1] A. Paghi, et al. *InAs on Insulator: A New Platform for Cryogenic Hybrid Superconducting Electronics.* Adv. Funct. Mater. 35, 7 (2025).

[2] A. Paghi, et al. Preprint (2024).

[P2.14] Thermal amplification in photonic heat transport based on Anderson insulators

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We present a device for controlling heat and temperature in the milliKelvin range, addressing a gap in state-of-the-art solid-state cryogenic technologies: the photonic heat amplifier (PHA) [1]. The PHA is centered around two Anderson insulator reservoirs connected by superconducting lines, enabling heat exchange through photonic modes [2]. The temperature sensitivity of the reservoir impedances enables the phenomenon of negative differential thermal conductance (NDTC), which can be employed to amplify oscillations of heat currents and temperatures in a thermal transistor configuration [3]. In the proposed device, one of the reservoirs is kept hot and acts as the source terminal of the transistor, while the gate and the drain consist of metallic reservoirs connected to the second Anderson element with tunnel contacts. In this setup, the heat flux from source to drain is controlled by the gate temperature. We present two distinct devices, each with optimized parameter choices, yielding different performances: the first focuses on amplifying small oscillations of the gate heat current on the source-drain flux, while the second manages to translate gate temperature variations into larger modulations of the temperature of the colder Anderson reservoir. Lastly, we present a design variation where all reservoirs are thermally connected through photonic modes, useful for controlling reservoirs distant in space. Our proposal answers to the lack of thermal transistors and amplifiers working at subKelvin temperatures, in a way that is also compatible with the advancements of circuit quantum electrodynamics. The PHA can contribute to various fields of quantum technologies, e.g,. sensing and the development of thermal circuits and control devices.

References

[1] M. Pioldi, G. D. Simoni, A. Braggio, and F. Giazotto. *Photonic heat amplifiers based on Anderson insulators.* arXiv:2502.04250 (2025).

[2] L. M. A. Pascal, H. Courtois, and F. W. J. Hekking. *Circuit approach to photonic heat transport.* Phys. Rev. B 83, 125113 (2011).

[3] B. Li, L. Wang, and G. Casati. *Negative differential thermal resistance and thermal transistor.* Appl. Phys. Lett. 88, 143501 (2006).

[P2.15] Linear response in proximity superconducting quantum interferometers

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Superconducting interferometers (SQUIDs) are quantum devices able to transduce a magnetic flux into an electrical output with excellent sensitivity, integrability and power consumption. Yet, their voltage response is intrinsically non-linear: a limitation which is conventionally circumvented through the introduction of compensation inductances or by the construction of complex device arrays, at the cost of a drastic reduction of the operation bandwidth. Here we discuss intrinsically linear flux-to-voltage mesoscopic transducers based on proximity Josephson junctions, either incorporated in bi-SQUIDs [1,2] or in double-loop superconducting quantum interference proximity transistors (SQUIPTs) [3]. We will show the low temperature performance of this these next generation quantum sensors based on aluminium and copper, and then discuss their temperature scalability using higher Tc materials such as Nb adn NbN.

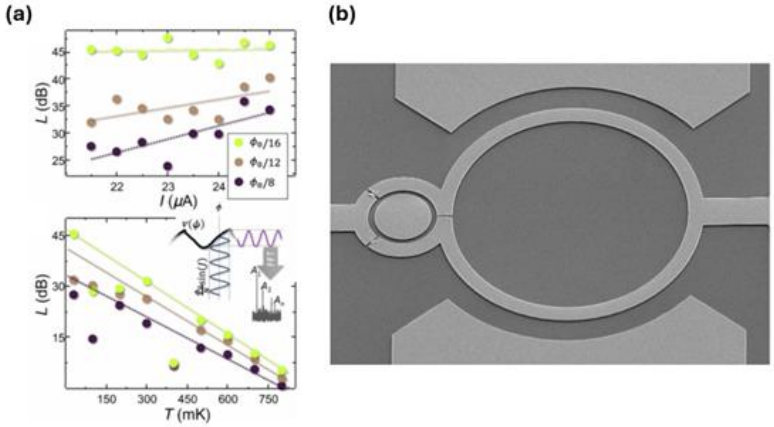

Fig. 1: (a) The linearity of the voltage-flux response of the □- □- □ bi-SQUIDs extracted from the experimental data of ref [1]. (b) Scanning electron micrograph of a double-loop dc superconducting quantum interference device (bi-SQUID) based on Nb superconductor–normal-metal–superconductor (□- □- □) proximity Josephson junctions.

References

[1] G. De Simoni, L. Cassola, N. Ligato, G. C. Tettamanzi, and F. Giazotto. *Ultrahigh Linearity of the Magnetic-Flux-to-Voltage Response of Proximity-Based Mesoscopic BiSQUIDs*. Phys. Rev. Applied 18, 014073 (2022).

[2] T. X. Kong, et al. Superconductor Science and Technology 37, 115014 (2024).

[3] G. De Simoni and F. Giazotto. *Ultralinear Magnetic-Flux-To-Voltage Conversion in Superconducting Quantum Interference Proximity Transistors.* Phys. Rev. Applied 19, 054021 (2023).

[P2.16] Tunable Superconducting Transport in 2D-InSb/Nb-based Hybrid Josephson Junctions with Dual-Gate Electrostatic Control

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Gate-tunable hybrid Josephson junctions provide a versatile platform for controlling superconducting transport, offering new opportunities for scalable quantum computing and superconducting logic applications. Here, we investigate dual gate electrostatic control on superconducting transport in 2D-InSb/Nb-based hybrid Josephson junction. We fabricate Josephson junctions on 2D-InSb nanoflags with the focus on top gate and bottom gate tunable supercurrent modulation. InSb nanoflags were grown using Au-assisted chemical beam epitaxy (CBE) on InP(111)B substrates [1]. A 300 nm thermally grown SiO_2 and 30 nm HfO_2 by atomic layer deposition are used as bottom and top gate dielectrics, respectively. The device, characterized at cryogenic temperatures (300 mK), exhibits clear multiple Andreev reflections (MAR) under varying voltage bias and gate control, indicating high junction transparency. Electrostatic gating via back gate voltage (varied between ±40 V) and top gate voltage (varied between ±4 V) demonstrates a clear modulation in the channel conductance, as shown in Fig.1. Systematic magnetic field sweeps from 0 to ±20 mT, at fixed back gate and top gate voltages, result in Fraunhofer patterns. As the back gate increases from 0V to 40V, the central lobe increases in amplitude, indicating an increase in the Josephson critical current, while the side lobes become more defined, suggesting higher coherence of supercurrent. Our results demonstrate an optimized experimental framework for engineering gate-controlled hybrid superconducting systems, relevant for quantum information processing and next-generation superconducting quantum circuits.

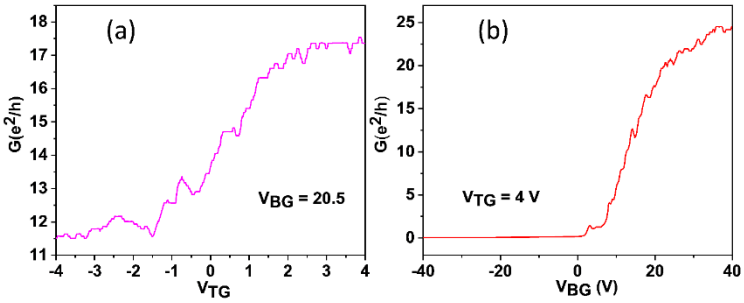

Fig. 1: Conductance modulation in a dual-gated 2D-InSb/Nb-based hybrid Josephson junction: (a) Conductance vs. top gate voltage at a fixed bottom gate voltage of 20.5 V, and (b) conductance vs. bottom gate voltage at a fixed top gate voltage of 4 V, at T = 4 K.

Reference

[1] I. Verma, S. Salimian, V. Zannier, S. Heun, F. Rossi, D. Ercolani, F. Beltram, and L. Sorba. *High-mobility free-standing InSb nanoflags grown on InP nanowire stems for quantum devices.* ACS Appl. Nano Mater. 4, 5825–5833 (2021).

[P2.17] Defect engineering of multilayer graphene with low energy Helium ion irradiation

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Ion irradiation has emerged as a powerful tool for engineering the properties of two-dimensional (2D) materials by introducing controlled defects [1]. Recent studies have demonstrated that precise ion irradiation can effectively tailor graphene's electronic and transport properties, making it highly relevant for applications in nanoelectronics, spintronics, and quantum materials [2]. The ability to control defect density and distribution enables fine-tuning of charge carrier mobility, band structure modifications, and even the emergence of novel quantum phenomena. Low-energy helium (He) ion irradiation provides a highly localized and controlled means of defect engineering while minimizing damage to the underlying substrate, making it particularly suited for targeted modifications in graphene-based devices [3]. In this study, monolayer, bilayer, and trilayer graphene samples were irradiated under high vacuum (1×10^{-7} mbar) with 1 keV He ions at varying doses, ranging from 1×10^{12} to 5×10^{13} ions/cm², to systematically investigate the largely unexplored layer-dependent defect dynamics.

Raman spectroscopy was employed to track the evolution of key spectral features, including intensity ratios (I_d/I_g, I_d/I_d') and peak widths (W_g, W_{2d}), providing insights into ion irradiation-induced disorder. To further interpret the experimental results, Monte Carlo simulations were conducted. Our findings reveal that He ion irradiation induces defects in graphene with density and characteristics strongly dependent on both the layer number and the ion dose. Monolayer graphene is particularly susceptible to ion exposure, exhibiting significant structural changes even at lower doses. With increasing ion dose, Raman spectra indicate heightened disorder, marked by the emergence and broadening of characteristic peaks, signalling a transition from a crystalline to an amorphous-like state at higher doses, in agreement with previous studies. In contrast, bilayer and trilayer graphene display more complex defect evolution, suggesting the formation of distinct defect structures influenced by interlayer interactions and ion scattering effects, as supported by Monte Carlo simulations.

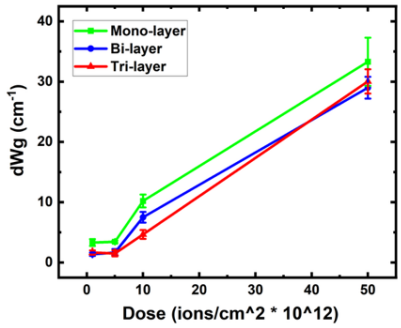

Fig.1: Mono-, bi-, and tri-layer graphene G-peak width change with the different He-ion dose.

References

[1] S. Kretschmer and A. V. Krasheninnikov. *Atomistic simulations of low energy ion irradiation of 2D materials: From ab-initio molecular dynamics to simple binary collision model.* Phys. Rev. Materials 8 (2024).

[2] M. Telkhozhayeva and O. Girshevitz. *Roadmap toward Controlled Ion Beam-Induced Defects in 2D Materials.* Adv. Funct. Mater 45 (2024).

[3] A. Eckmann, A. Felten, A. Mishchenko, L. Britnell, R. Krupke, K. S. Novoselov, and C. Casiraghi. *Probing the Nature of Defects in Graphene by Raman Spectroscopy.* Nano Lett. 12 (2012).

[P2.18] Supercurrent diodes, from fundamental physics to future quantum technologies

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A superconducting diode enables supercurrent to flow in only one direction, providing new functionalities for superconducting circuits. In recent years, significant experimental progress has been made towards realizing such behavior in both Josephson junctions and superconducting films. This presentation reviews the experimental work and theoretical developments of the superconducting diode effect (SDE) [1], focusing on the main activities developed at Cnr Nano.

The observation of the SDE is discussed, including material realization, device geometry, and experimentally measured parameters, reflecting the presence of non-reciprocity through the lens of symmetry breaking. Various platforms are presented, ranging from strong spin–orbit Al Josephson junctions made of InAs and InSb [2] to more exotic bilayers of Al/$NiBr_2$. In the latter, the SDE reveals helical superconductivity engineered through the magnetic proximity effect of the van der Waals $NiBr_2$ layer and controlled by external magnetic fields, revealing the non-trivial conical spin pattern on the $NiBr_2$ surface [3].

Additionally, it is shown how back-action can be exploited to achieve non-reciprocal transport in reciprocal superconducting circuits, enabling the design of gate-controlled diodes that form the basis of novel diode-based superconducting logic[5] and rectifiers. Finally, a perspective on future directions in this active research field is provided, analyzing electric field tunability and discussing the emergent topological superconducting technologies.

References

[1] M. Nadeem, M.S. Fuhrer, and X. Wang. *The superconducting diode effect.* Nat. Rev. Phys. 5(10), 558–577 (2023).
[2] B. Turini, S. Salimian, M. Carrega, A. Iorio, E. Strambini, F. Giazotto, V. Zannier, L. Sorba, and S. Heun. *Josephson Diode Effect in High-Mobility InSb Nanoflags*. Nano Lett. 22(21), 8502–8508 (2022).
[3] D. Amoroso, P. Barone, and S. Picozzi. *Spontaneous skyrmionic lattice from anisotropic symmetric exchange in a Nihalide monolayer*, Nat Commun 11(1), 5784 (2020).
[4] D. Margineda, A. Crippa, E. Strambini, L. Borgongino, A. Paghi, G. De Simoni, L. Sorba, Y. Fukaya, M.T. Mercaldo, C. Ortix, M. Cuoco, and F. Giazotto. *Back-action supercurrent rectifiers.* Commun Phys 8(1), 1–7 (2025).
[5] P. Hosur. *Digital logic from high-efficiency superconducting diodes.* Preprint (2024).

Project

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[P2.19] Heat-charge separation in hybrid superconducting systems

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Separating heat from charge in a material is an extremely challenging task since they are transported by the very same carriers, i.e., electrons or holes, and requires the violation of the Wiedemann-Franz law. On the other hand, controlling independently heat and charge flows can greatly enhance thermoelectric performances of a heat engine at low temperatures. In a multiterminal device the heat and charge currents can, however, follow different paths. In this talk I will introduce and analyze a class of multiterminal devices where this property is pushed to its extreme limits, with charge and heat currents flowing in different reservoirs [1]. In particular, I will show that such separation can reach 100% efficiency in a hybrid superconducting quantum Hall setup, provided that the quantum Hall system is tuned to integer filling factor, see Fig. 1. We present microscopic calculations for a three-terminal setup to illustrate our idea [2].

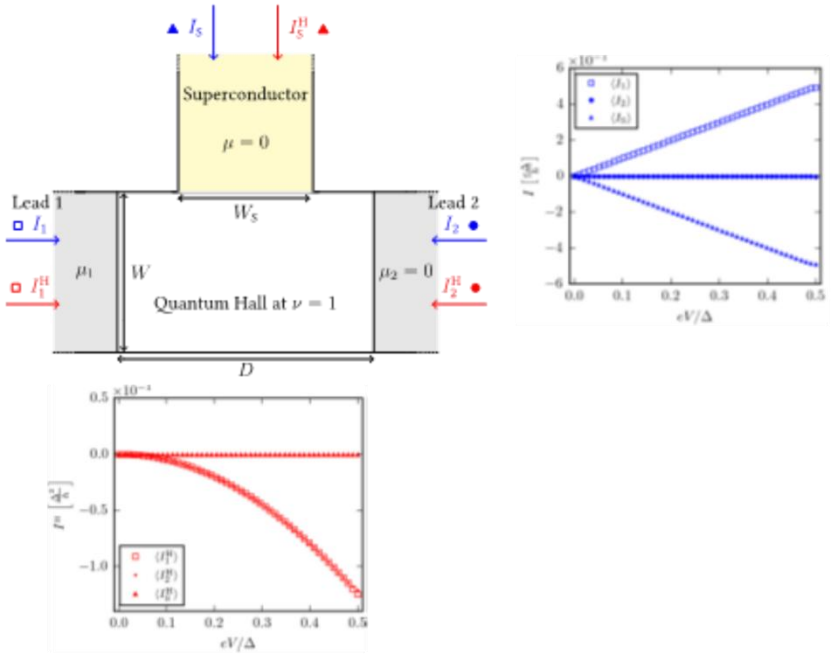

Fig. 1: Quantum Hall/Superconductor setup (left), charge (middle) and heat (right) currents.

References

[1] F. Mazza, S. Valentini, R. Bosisio, G. Benenti, V. Giovannetti, R. Fazio, and F. Taddei. *Separation of heat and charge currents for boosted thermoelectric conversion*. Phys. Rev. B 91, 245435 (2015).

[2] C. Panu, F. Taddei, M. Polini, and A. Yacoby. *Heat-charge separation in a hybrid superconducting quantum Hall setup.* Phys. Rev. B 110, L161407 (2024).

[P2.20] Genuine multipartite entanglement from many-electron systems

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We demonstrate that, contrary to common wisdom, genuine multipartite entanglement (GME) can be abundantly generated from simple non-correlated many-electron states. We show that the extracted GME can be maximized via spin-independent transformations derived from the quantum Fourier transform. We further demonstrate the possibility of maximizing the GME through localized orbitals in a variety of realistic systems and correlated states. Towards the exploitation of potentially useful entanglement, we rationalize system-specific and universal features of the extracted GME [1].

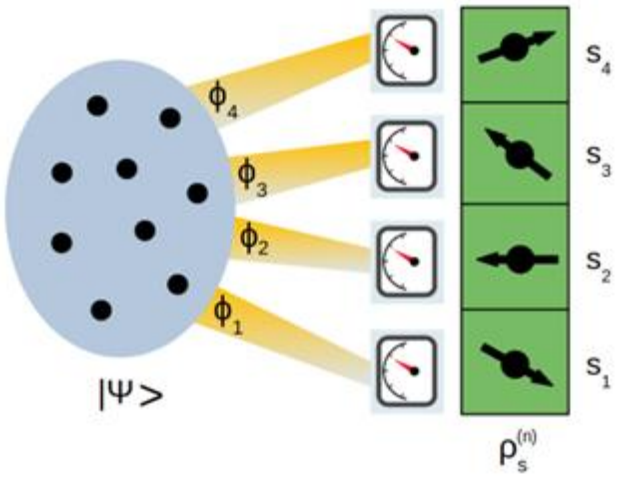

Fig. 1: Schematic representation of the considered procedure: *n* particles (here *n*=4) are detected from an N-electron state |Ψ>. The spins s_i, whose entanglement properties we investigate, are identified through the orbitals (or detection modes) ϕ_i .

Reference

[1] F. Troiani, C. Angeli, A. Secchi, and S. Pittalis. *Genuine multipartite entanglement from many-electron systems.* arXiv:2410.11314 (2024).

[P2.21] A quasiparticle-injection superconducting microwave relaxation oscillator: the QUISTRON

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We introduce the QUISTRON [1], a superconducting microwave relaxation oscillator comprising a nanowire shunted by a resistor and inductor, with frequency tunable through quasiparticle injection from a tunnel junction. Operating via localized heating that modulates the nanowire switching current, this device demonstrates voltage-controlled frequency tuning in the 1-10 GHz range with remarkably low energy consumption (~100 zJ per cycle). Our simulations across various parameters such as shunt resistance, inductance, and bath temperatures from 20 mK to 1 K confirm robust performance. The QUISTRON simple frequency control mechanism and integration potential make it particularly suitable for quantum information processing, microwave applications, and ultralow-power electronics as a compact, tunable superconducting local oscillator.

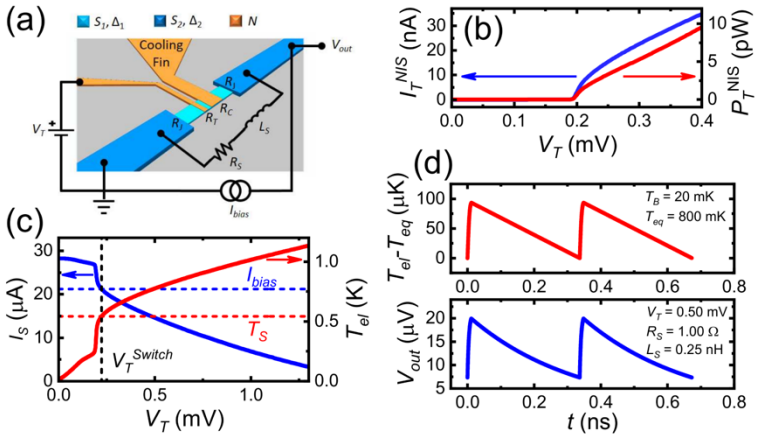

Fig. 1: The QUISTRON is a superconducting nanowire device that generates GHz-range oscillations through thermal cycling. a) Circuit scheme: A superconducting nanowire (S_1) shunted by R_S and L_S connects to superconducting banks (S_2) via tunnel junctions. Additional junctions (R_T, R_C) enable quasiparticle injection and cooling through a normal metal contact and cooling fin. b) NIS junction characteristics: Charge and heat currents versus V_T at T_B = 20 mK, showing insulating behavior below the gap voltage (Δ_1/e = 0.2 mV). c) Nanowire switching current and electronic temperature versus V_T, demonstrating sharp IS drop at $V_T \simeq \Delta_1/e$ due to increased heating. Dashed lines indicate bias values and switching parameters. d) Simulated temperature and voltage oscillations (V_T = 0.50 mV, T_B = 20 mK) showing nanowire switching between normal and superconducting states, producing 3 GHz oscillations.

Reference

[1] G. Trupiano, G. De Simoni, and F. Giazotto. *Quasiparticle-injection superconducting microwave relaxation oscillator.* Phys. Rev. Appl. 23, 014046 (2025).

[P2.22] Modifications induced by H_2 and H_2O exposure on Cu-doped cerium oxide films by X-ray Absorption Spectroscopy at ambient pressure

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Cerium oxide is a relevant material in catalysis due to the relative stability of Ce cations in two oxidation states, 4+ and 3+, and to the related ability to reversibly store and transport O atoms. The replacement of a minority of Ce cations with lower-valence metal ions was shown to decrease the O vacancy formation energy and the catalytic activity of the material. Interesting applications of cerium oxide-based materials can be found in hydrogen-related technologies, where they are used as electrodes in photoelectrochemical cells for hydrogen conversion – fuel cells – and for hydrogen generation by water photoelectrolysis.
To unravel the specific mechanisms that determine the functionality of Cu-doped ceria in such devices, we have employed X-ray absorption near-edge spectroscopy (XANES) under ambient H_2 and H_2O pressure on films with different doping concentrations. The measurements were performed at the APE-HE beamline of the ELETTRA synchrotron radiation source, using a reaction cell with an ultrathin membrane that confines the gas flux in a narrow region extremely close to the sample surface. Ce M_{45}-edge and Cu L_{23}-edge spectra were measured during thermal treatments in H_2 and H_2O at ambient pressure. Gas chromatography was used to correlate the observed spectroscopic modifications with the chemical activity of the materials.
Pure ceria showed a progressively increasing relative intensity of the Ce^{3+}-related features with increasing temperature in H_2 pressure (Fig. 1a). In Cu-doped films, as the Cu concentration increases, the same treatment led to a progressively higher intensity of the Ce^{3+}-related features (Fig. 1b and c). This evidence, combined with the evolution of the Cu oxidation state and with gas chromatography, suggested that at moderate temperatures H_2 dissociation is favored by the presence of Cu^{1+} sites, and at higher temperature water is desorbed from the surface with the uptake of oxygen from cerium oxide [1].
The modifications of the same materials upon H_2O exposure and the effect of irradiation with laser light at 375 nm wavelength were also investigated. Also in this case the Cu dopant ions were found to be active in modifying the electronic structure of CeO_2, and in enabling more efficient hydrogen production at lower temperatures, as compared to the pure oxide [2].

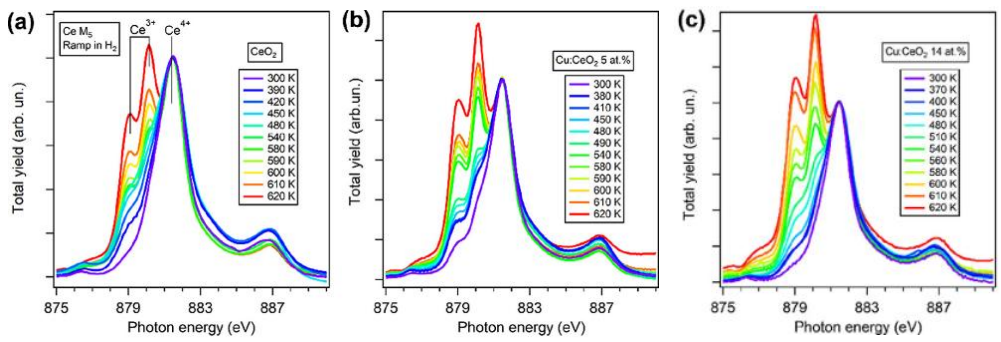

Fig. 1: Ce M_5-edge XANES spectra of (a) undoped CeO_2 (b) a Cu:CeO_2 5 at. % doped film and (c) a Cu:CeO_2 14 at. % doped film acquired at different T in H_2 at ambient pressure

References

[1] A. Vikatakavi, et al. *Role of Metal Dopants in Hydrogen Dissociation on Cu:CeO_2 and Fe:CeO_2 Surfaces Studied by Ambient-Pressure X-ray Absorption Spectroscopy.* ACS Appl. En. Mater. 7, 2746-2754 (2024).
[2] E. Spurio et al. In preparation.

[P2.23] Quantitative detection of olive polyphenols by QCM using bio-derived functional polymers

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In recent years, there has been an increasing interest in bio-derived polymers due to their sustainability, eco-friendliness, and potential to replace conventional petroleum-based materials. These bio-based polymers are derived from renewable resources, making them an attractive alternative in various industries, particularly in the context of environmental concerns. Their biodegradability, lower carbon footprint, and reduced reliance on fossil fuels contribute significantly to reducing environmental impact, aligning with the global drive towards greener technologies and sustainable practices [1]. One of the most promising aspects of bio-derived polymers is their versatility, which allows for functionalization to enhance their performance in various applications.

The main objective of this work is to explore the development of novel bio-derived materials, with a focus on their application as functional layers in Quartz Crystal Microbalance (QCM) sensors. QCM sensors are highly sensitive devices used for detecting mass loading, making them ideal for a variety of applications, including environmental monitoring, chemical sensing, and biosensing. By developing functional bio-derived polymers as QCM active layers, we aim to enhance the performance of these sensors, particularly in the detection of polyphenols.

Polyphenols are a class of bioactive compounds widely found in plant-based foods and beverages, such as fruits, vegetables, oil, tea, and wine. They are known for their antioxidant properties and health benefits, and their content can be a ripeness indicator for fruits and a quality marker for their final derivatives [2]. However, their detection in complex matrices requires sensitive and selective analytical techniques. By utilizing modified chitosanic and cellulosic polymers as functional layers in QCM sensors, we aim to create an efficient, eco-friendly, and cost-effective method for detecting polyphenols in vegetables, with specific attention for olive extracts. The polymeric layer will interact with the polyphenols, resulting in measurable changes in the QCM sensor's frequency response, which can then be used to quantify the polyphenol concentration. This work explores the potential for creating a more sustainable and green approach to analytical sensing technologies, aligning with the growing demand by food and agricultural industry for environmentally friendly solutions.

References

[1] A. K. Mohanty, F. Wu, R. Mincheva, M. Hakkarainen, J. M. Raquez, D. F. Mielewski, R. Narayan, A. N. Netravali, and M. Misra. *Sustainable polymers.* Nature Reviews Methods Primers 2, 46 (2022).

[2] F. A. Tomás-Barberán and J. C. Espín. *Phenolic compounds and related enzymes as determinants of quality in fruits and vegetables.* Journal of the Science of Food and Agriculture 81, 853 (2001).

Project

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[P2.24] Humidity-Resistant Ultra-Low Friction in DLC Coatings Enabled by Graphitic Nanodiamonds

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Diamond-like carbon (DLC) coatings are widely used in tribological applications due to their low friction, high wear resistance, and chemical stability [1, 2]. The pursuit of ultra-low friction, quantified with a coefficient of friction (CoF) below 0.1, has led to DLC functionalization with nanomaterials. Studies have indicated that nanodiamonds (NDs) combined with graphene enabled macroscale superlubricity in dry conditions via *in situ* graphene nanoscroll formation [3]. However, this approach struggles in humid environments and requires peculiar conditions, such as multi-step processing and ultra-flat substrates. In our previous work [4], we achieved ultra-low friction on industrially micro rough DLC coatings using a synergistic combination of commercial graphene flakes (GFs) and NDs, though only in dry conditions. Here, we introduce a single-step functionalization using Graphitic Nanodiamonds (Gr-NDs), pre-synthesized core-shell nanostructures with nanodiamond cores wrapped in few-layer graphene. Tribological tests both in humid air (50–60% R.H.) and in dry nitrogen confirm that Gr-NDs enable stable ultra-low friction, overcoming humidity-related limitations. Raman spectroscopy, TEM, and EELS analyses reveal the direct incorporation of Gr-NDs into a lubricating transfer layer, ensuring friction reduction and wear resistance, which is not achieved by using nanostructures without core-shell architecture. This scalable approach offers a simple and effective solution for industrial applications, expanding the potential of DLC coatings under real-world conditions.

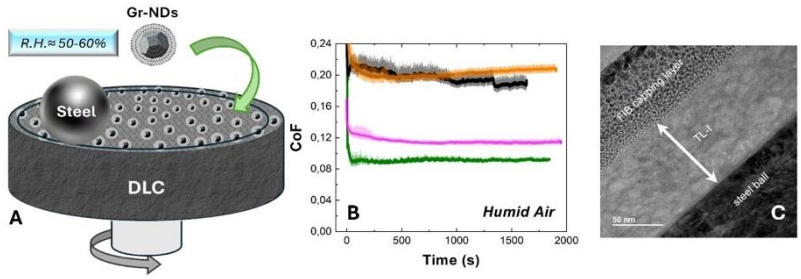

Fig. 1: A) Not-to-scale scheme diagram of tribological test performed in humid environment on DLC substrate functionalized with Graphitic Nanodiamonds (Gr-NDs). B) CoFs plots as a function of time of DLC substrate functionalized through different carbon nanostructures. C) HRTEM image from the cross-sectional sample of the transfer layer.

References

[1] S.K. Field, M. Jarratt, and D. G. Teer. *Tribological properties of graphite-like and diamond-like carbon coatings.* Tribology International 37, 949–956 (2004).

[2] A. Erdemir and O. Eryilmaz. *Achieving superlubricity in DLC films by controlling bulk, surface, and tribochemistry.* Friction 2, 140–155 (2014).

[3] D. Berman, S.A. Deshmukh, S. K. R. S. Sankaranarayanan, A. Erdemir, and A.V. Sumant. *Macroscale superlubricity enabled by graphene nanoscroll formation.* Science 348, 1118–1122 (2015).

[4] A. Mescola, A. Lodi, F. Zanni, A. Rota, A. Gerbi, C. Bernini, M. Schott, L. Repetto, A. Camisasca, S. Giordani, R. Buzio, and G. Paolicelli. *Synergistic effect of graphene and nanodiamonds to achieve ultra-low friction on rough DLC coatings.* Diamond and Related Materials 145, 111149 (2024).

[P2.25] Harvesting blue energy using piezoelectric nanogenerators

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Scavenging kinetic energy from sea currents and sea waves (blue energy) is nowadays one of the most promising and attractive renewable energy. Recent estimations [1] highlight that the average wave energy along the world's coasts is approximately 40 MW per km, and sea currents are particularly relevant in this context since they are highly predictable and widely distributed. Energy harvesting devices can exploit such kinetic energy to generate currents and voltages that, in turn, can be used to provide a stable and continue power supply to a distributed network of marine sensors. Among parameters of interest that can be monitored, there are temperature, pH, turbidity, pressure, and chemical substances such as chlorophyll, nitrate andoxygen.

In terms of generated power density and output voltages, electromagnetic and triboelectric energies are the most promising sources, although an interesting alternative is represented by piezoelectricity which in a device configuration offers mechanical advantages in terms of flexibility, low-cost manufacturing processes and reduced lateral size and thickness.

In the framework of the Italian "Piano Nazionale di Ripresa e Resilienza (PNNR)", mission 4, the objects of "NEST – Network 4 Energy SustainableTransition"aims at "building a competent Italian leadership, consistent with existing excellence of the partners and affiliates, capable of supporting the growth of new generation of energy technologies, researchers and research infrastructures for a future sustainable and resilient energy sector is the exploitation of natural energy sources, such as wind and marine waves for the development of off-shore renewables as well as novel energy harvesting technologies."

In this context, our research activity aims at the development of innovative devices by harvesting energy from vibrations/mechanical displacements by exploiting piezoelectricity.

Here we present a simple, flexible device architecture consisting of an active piezoelectric layer sandwiched between two metal electrodes (Fig. 1a) designed for harvesting blue energy. The active layer consists of a mat of nanofibers (Fig. 1b) composed of both polymeric and inorganic compounds. Different approaches were developed to improve the device performance in terms of generated voltage and power density and several device architectures were designed to obtain a soft and flexible device with high operational stability both in air and in water and to build safe external connection for the collection of the voltage and current generated.

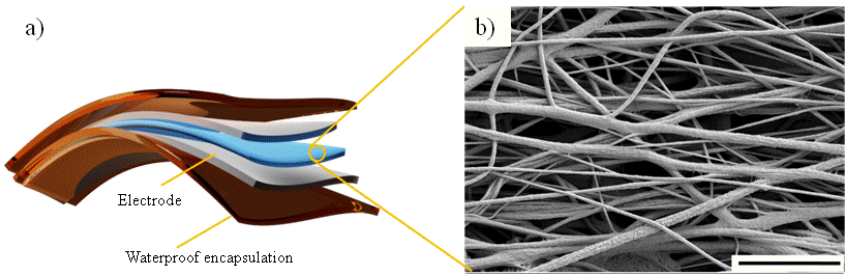

Fig. 1: a) Schematic of the piezoelectric device developed and b) scanning electron micrograph of piezoelectric nanofibers. Scale bar: 10µm.

Project
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[P2.26] AI-enhanced electron microscopy

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In this talk, we explore the transformative impact of Artificial Intelligence (AI) on Transmission Electron Microscopy (TEM) and its emerging role in revolutionizing both experimental design and data analysis. Recent advances have enabled the integration of external stimuli into the microscope environment through interoperable systems and Micro-Electro-Mechanical Systems (MEMS) technology. These innovations not only facilitate the incorporation of custom optics and miniaturized devices for in situ and in operando experiments but also set the stage for a new generation of adaptive, AI-enabled instruments.

The increasingly sophisticated experimental setups generate vast, high-resolution datasets that challenge traditional data acquisition and processing methods. AI, particularly through the application of neural networks (NNs), has become indispensable in addressing these challenges. Modern neural network architectures are now capable of performing complex pattern recognition, predictive modelling, and real-time analysis at speeds that far exceed human capabilities. These tools enable dynamic adjustments and optimization during experiments, ensuring precision and consistency even in prolonged, high-throughput studies.

Moreover, advances in remote and cloud-based processing are paving the way for fully integrated workflows. Automated analysis tools [1] now facilitate tasks such as diffraction pattern interpretation, elemental quantification, and large-scale data mining, streamlining the pathway from data collection to scientific insight. As these systems mature, the role of AI in reducing measurement redundancy, anticipating experimental outcomes, and guiding decision-making processes becomes ever more critical [2].

By showcasing current applications of AI in TEM and highlighting recent breakthroughs in workflow automation and remote processing, we envision a future where human expertise and artificial intelligence work in seamless collaboration. This synergistic partnership not only promises to push the boundaries of discovery in the microscopic realm but also heralds a new era of innovation and efficiency in scientific exploration.

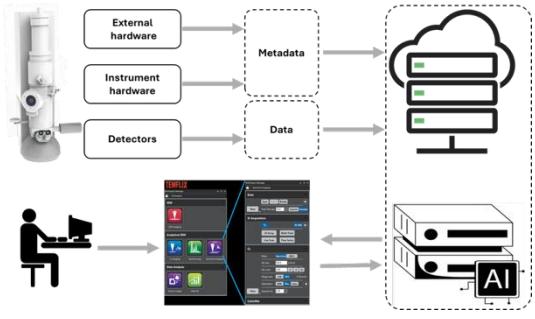

Fig. 1: Schematic of an AI-powered, cloud-integrated TEM workflow: Experimental data and metadata from the TEM, including detectors and external hardware, are transmitted to cloud storage for remote access. Users interact with analysis software, leveraging AI-driven tools for automated data interpretation and decision-making.

References

[1] M. Botifoll, et al. *Artificial Intelligence End-to-End Workflow for Transmission Electron Microscopy: From Data Analysis Automation to Materials Knowledge Unveiling.* arXiv:2411.0102 (2024).

[2] N. R. Lewis, Y. Jin, X. Tang, V. Shah, C. Dotty, B. E. Matthews, S. Akers, and S. R. Spurgeon. *Forecasting of in situ electron energy loss spectroscopy.* npj Comput. Mater. 8, 252 (2022).

[P2.27] Anisotropic rheology and friction of suspended graphene

A. Mescola[1], A. Silva[2,3], A. Khosravi[3,4], A. Vanossi[2,3], E. Tosatti[3,4], S. Valeri[5,1], and G. Paolicelli[1]

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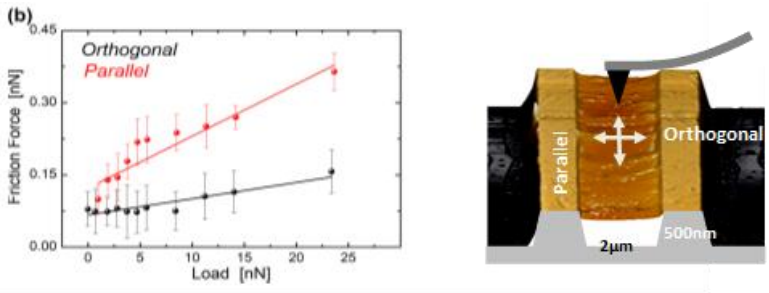
Graphene is a powerful membrane prototype for both applications and fundamental research [1,2]. Rheological phenomena including indentation, twisting, and wrinkling in deposited and suspended graphene are actively investigated to unravel the mechanical laws at the nanoscale. Most studies focused on isotropic setups, while realistic graphene membranes are often subject to strongly anisotropic constraints, with important consequences for the rheology, strain, indentation, and friction in engineering conditions. Graphene is recognized as the thinnest solid lubricant material and a large amount of work has been dedicated to understanding the fundamentals mechanisms of this effect and to unravel parameters relevant to its technological development. Here, we experimentally show how graphene's frictional response to an external indenter is severely altered by conditions of anisotropic suspension, specifically when graphene is clamped across a long and narrow groove. Results show that the friction coefficient is significant when the tip is sliding parallel to the groove while becoming ultralow in the orthogonal direction. While the experimental data suggest that, rather unexpectedly, pre-strain of the graphene sheet as a result of clamping is negligible, the key to understanding the underlying mechanism is provided by simulations. The paramount mechanism is provided by the extra anisotropic strain induced from indentation under anisotropic constraints, which in turn produces an anisotropic stiffening of the graphene. While the focus of this work is on graphene, we believe our experimental protocol and the physical mechanism uncovered by our model can be applicable to other 2D membrane like materials.



References
[1] A. Mescola, A. Silva, A. Khosravi, A. Vanossi, E. Tosatti, S. Valeri, and G. Paolicelli. *Anisotropic rheology and friction of suspended graphene.* Physical Review Materials 7, 054007 (2023).
[2] A. Mescola, G. Paolicelli, S. P. Ogilvie, R. Guarino, J. G. McHugh, A. Rota, E. Iacob, E. Gnecco, S. Valeri, N. M. Pugno, V. Gadhamshetty, M. M. Rahman, P. Ajayan, A. B. Dalton, and M. Tripathi. *Graphene confers ultralow friction on nanogear cogs.* Small 17, 2104487 (2021).
[3] M. Liu, Z. Li, X. Zhao, R. J. Young, and I. A. Kinloch. *Fundamental insights into graphene strain sensing.* Nano Lett. 21, 833 (2021).
[4] S. Zhang, Y. Hou, S. Li, L. Liu, Z. Zhang, X.-Q. Feng, and Q.Li. *Tuning friction to a superlubric state via in-plane straining.* Proc. Natl. Acad. Sci. USA 116, 24452 (2019).

[P2.28] A procedure to obtain niobium oxide films with variable stoichiometry

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Niobium oxide films display noteworthy optical and electrical characteristics, making them suitable for various technological applications. Niobium oxides have three relatively stable stoichiometries: NbO, NbO_2, and Nb_2O_5. Of these, Nb_2O_5 is the most thermodynamically stable phase and is used as a photocatalyst due to its strong redox ability, as well as in Li-ion batteries. NbO is a conductive oxide exhibiting superconductive behavior at 1.38 K and is used in capacitors in combination with Nb_2O_5 as a dielectric. NbO_2 undergoes a thermally induced insulator-to-metal transition (IMT) at 810°C, which can also be triggered by light absorption. This sudden change in conductivity makes it suitable for applications in memristive devices, ultrafast electrical switches, and thermal sensors.

Previous research has primarily concentrated on the growth of niobium oxide films with specific stoichiometries. In particular, physical synthesis methods have been employed to produce films with thicknesses ranging from several tens to several hundreds of nanometers. However, maintaining a high degree of control over the stoichiometry during the growth process and achieving various stoichiometric phases has proven to be quite challenging.

This study introduces a novel procedure for fabricating niobium oxide films and fine-tuning their stoichiometry among the three most stable oxide phases. Starting with a magnetron-sputtered film predominantly composed of Nb_2O_5, its structure and stoichiometry are optimized through thermal treatment in an O_2/N_2 flux. A vacuum reduction treatment transforms the as-grown film into the NbO phase, which can then be re-oxidized under controlled oxygen partial pressure to achieve the NbO_2 phase. Furthermore, a comprehensive characterization of the three different niobium oxides in terms of structure, optical properties, morphology, and surface composition is presented. Additionally, the NbO_2 films are characterized using Femtosecond Transient Absorption Spectroscopy (FTAS) to investigate the photoinduced insulator-to-metal transition (IMT). This analysis explores how ultrafast dynamics are influenced by excitation energy and intensity and discusses the observed ultrafast transient absorbance in relation to recent research findings [1].

The obtained results serve as a reference for future studies on the dynamics of light-induced processes using element-sensitive ultrafast X-ray techniques. As an initial step in this direction, we present and discuss X-ray absorption near-edge spectroscopy (XANES) measurements at the Nb K edge, which were performed on some of the films with ultrashort high-energy photon pulses generated by the European X-ray Free Electron Laser (EuXFEL). The feasibility of these high-energy measurements, which provide precise information on the electronic properties of the films, opens up new possibilities for investigating light-induced processes in the studied materials.

Reference

[1] S. Pelatti, S. Benedetti, G. Ammirati, P. O' Keeffe, D. Catone, S. Turchini, X. Huang, Y. Uemura, F. Lima, C. J. Milne, and P. Luches. *Niobium oxide films with variable stoichiometry: structure, morphology and ultrafast dynamics.* J. Phys Chem C, in press (2025).

[P2.29] Using Phase Retrieval Techniques at Cnr Nano/UNIMORE to Study magnetic and electric fields at the nanoscale.

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Phase retrieval techniques in electron microscopy have significantly advanced our ability to probe materials and biological specimens at the atomic scale, offering insights into electromagnetic fields, electrostatic potentials, and structural characteristics of samples. Among these techniques, Differential Phase Contrast (DPC), the Transport of Intensity Equation (TIE), Off-Axis Electron Holography and Electron Ptychography have emerged as pivotal methodologies, each with unique principles and applications.

Each of these techniques presents distinct advantages and challenges. Differential Phase Contrast (DPC) microscopy exploits the interaction between the electron beam and electromagnetic fields in a specimen, enabling the mapping of phase shifts induced by local electric and magnetic fields [1]. It is one of the ideal methods for investigating magnetic domain structures, electric field distributions in semiconductor devices, and charge density mapping in functional materials. The Transport of Intensity Equation (TIE) [2] approach leverages the relationship between the intensity variations along the propagation direction of the electron beam and the phase of the electron wavefront. TIE-based methods have been widely used in the study of weak-phase objects, including biological specimens and low-Z materials. Nevertheless, accurate phase retrieval in TIE requires precise defocus calibration and may be limited by the presence of noise and non-linear phase contributions, which complicate the inversion process. Off-Axis Electron Holography [3], on the other hand, directly encodes phase information by interfering a reference electron wave with the object wave. This method offers unparalleled precision in phase measurements, enabling the investigation of electric and magnetic fields at the nanometer scale, quantification of electrostatic potentials in semiconductor devices, and probing of charge distributions in quantum materials. Ptychography [4,5] is a computational imaging technique that reconstructs both the amplitude and phase of the electron wave by processing a series of overlapping coherent diffraction patterns obtained by scanning the specimen. Ptychography offers high-resolution phase imaging and has been applied to a variety of specimens, including biological samples and two-dimensional materials.

The choice of phase retrieval technique depends on the specific scientific question, the nature of the sample, the desired spatial and phase resolution. Here in Modena, we can perform DPC, TIE and Off-Axis Holography at either the new SPEQTEM microscope or at the TEM present in the CIGS. Future upgrades of the new SPEQTEM microscope may also allow us to perform electron ptychography experiments.

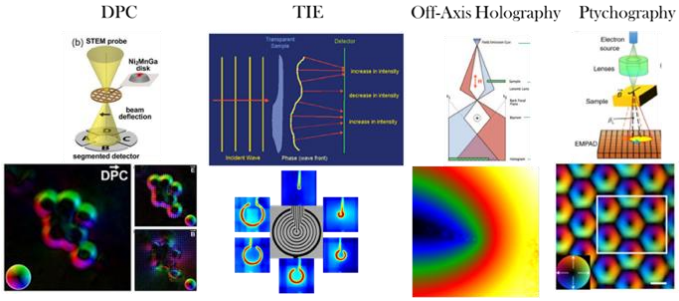

Fig. 1: Schematic representation for the four techniques for phase retrieval. For each technique the top row shows the working principle, while the bottom row shows experimentally retrieved phases. For DPC and Ptychography the experimental phases have been taken from [1] and [5] respectively.

References

[1] M. Campanini, et al. Appl. Phys. Lett. 117 (2020).
[2] K. Ishizuka and B. Allman. Micros. Today 13, 22–5 (2005).
[3] G. Pozzi. Advances in Imaging and Electron Physics 194, 245–69 (2016).
[4] Y. Jiang, et al. Nature 559, 343–9 (2018).
[5] Z. Chen, et al. Nat. Nanotechnol. 17, 1165–70 (2022).

[P2.30] Epitaxial 3D graphene on porous 4H-SiC(0001): a promising platform for hydrogen storage and sensing applications

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Porous materials represent a versatile solution in many fields ranging from materials science to biomedical applications. The possibility of combining the outstanding properties of epitaxial graphene to a porous structure is, therefore, extremely promising. Indeed, the successful growth of high-quality epitaxial graphene (3DG) on porousified crystalline 4H-SiC(0001) has been recently achieved [1]. The porousified layer is about 20 □m thick, and its pores are interconnected. They have an average diameter of around 100 nm. Graphene covers the walls of the pores of the entire porous layer. The pristine 3DG has been characterized and successively assessed for hydrogen storage application [2] and sensing [3].
Several investigations, both theoretical and experimental, have demonstrated that metal functionalization can tailor and enhance the graphene interaction with hydrogen. While the metal decoration of flat epitaxial graphene can be easily performed *in situ* with commercial evaporators/dispensers, the functionalization of a porous material is not as straightforward. We have successfully explored the *ex-situ* functionalization with metal nanoparticles (NPs) by immersing the sample in a colloidal solution of NPs [4]. Indeed, the NPs can penetrate down to the bottom of the porous layer, while they are preserved from oxidation by the organic capping layer utilized during the synthesis [5]. The interaction of 3DG with the NPs has been investigated by X-ray Photoelectron Spectroscopy (XPS), in a wide temperature range. Hydrogenation experiments have demonstrated the connection of some of the desorption peaks with the active sites of the sample.

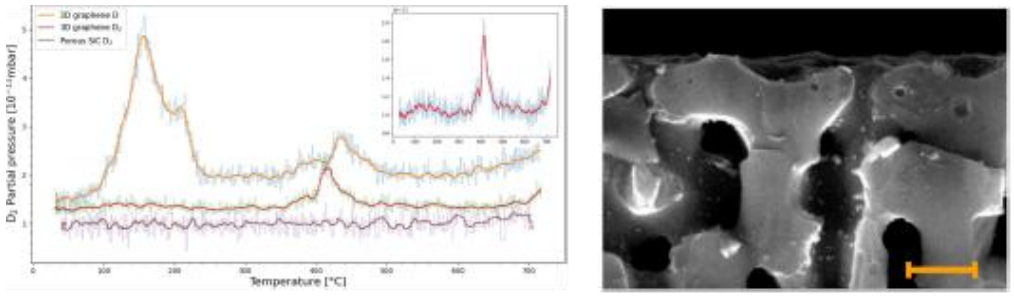

Fig. 1: (a) Temperature desorption spectra after hydrogenation of a pristine 3DG sample. (b) Cross-sectional SEM image of a 3DG sample functionalized with Pd NPs. Scale bar 200 nm.

References

[1] S. Veronesi, et al. *3D arrangement of epitaxial graphene conformally grown on porousified crystalline SiC.* Carbon, 189, 210–218 (2022).
[2] A. Macili, et al. *Study of hydrogen absorption in a novel three-dimensional graphene structure: Towards hydrogen storage applications.* Applied Surface Science 615, 156375 (2023).
[3] S. Veronesi, et al. *Three-dimensional graphene on a nano-porous 4H-SiC backbone: a novel material for food sensing applications.* J. Sci. Food Agric. 105, 1413-1419 (2025).
[4] E. Pompei, et al. *Functionalization of three-dimensional epitaxial graphene with metal nanoparticles.* Nanoscale 16, 16107-16118 (2024).
[5] Y. Vlamidis, et al. *Rapid synthesis of uniformly small nickel nanoparticles for the surface functionalization of epitaxial graphene.* Part. Part. Syst. Charact. 41, 2400141 (2024).

[P2.31] Magnetic Transparent Conductors for Spintronics

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Transparent Conductors (TCs) exhibit optical transparency and electron conductivity and are essential for many opto-electronic and photo-voltaic devices. The most common TCs are electron-doped oxides, which are limited in the choice of possible dopants, as transition metals most often are not suitable, in wiev of their tendency to form strong oxygen bonds. Non-oxides TCs have the potential of extending the class of materials to the magnetic realm, bypass technological bottlenecks, and bring TCs to the field of spintronics. Here we propose new functional materials that combine transparency and conductivity with magnetic spin polarization that can be used for spintronic applications, such as spin filters. By using high-throughput first-principles approaches [1, 2, 3], we identified many potential TCs, including non-oxides materials. Our results indicate that proper doping with transition metals introduces a finite magnetization that can provide spin filtering up to 90% in the electrical conductivity, still maintaining a transparency greater than 90% [4].

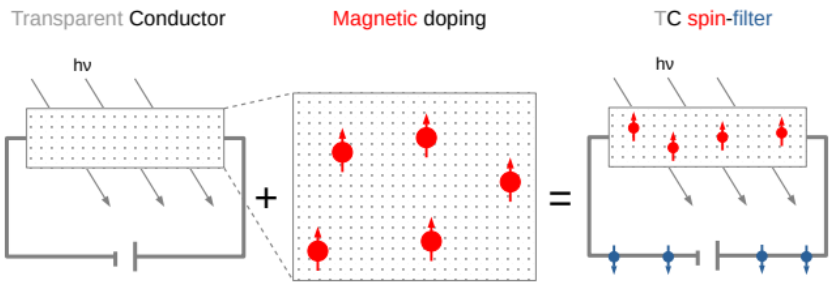

Fig. 1: Graphical representation of the identification of potential transparent conductor spin-filter.

References

[1] P. D'Amico, L. Agapito, A. Catellani, A. Ruini, S. Curtarolo, M. Fornari, M. Buongiorno Nardelli, and A. Calzolari. *Accurate ab initio tight-binding Hamiltonians: Effective tools for electronic transport and optical spectroscopy from first principles.* Phys. Rev. B 94, 165166 (2016).

[2] A. R. Supka, T. E. Lyons, L. Liyanage, P. D'Amico, R. Al Rahal Al Orabi, S. Mahatara, P. Gopal, C. Toher, D. Ceresoli, A. Calzolari, S. Curtarolo, M. Buongiorno Nardelli, and M- Fornari. *AFLOWπ*: *A minimalist approach to high-throughput ab initio calculations including the generation of tight-binding hamiltonians.* Comp. Mater. Sci. 136, 76-84 (2017).

[3] P. Giannozzi, et al. *Advanced capabilities for materials modelling with Quantum ESPRESSO.* J. Phys. Cond. Mat. 29, 465901 (2017).

[4] P. D'Amico, A. Catellani, A. Ruini, S. Curtarolo, M. Fornari, M. Buongiorno Nardelli, and A. Calzolari. *Magnetic transparent conductors for spintronic applications.* Acta Materialia 289, 120850 (2025).

[P2.32] Machine Learning-Accelerated DFT Conformal Sampling of Activated Processes in Catalysis and Materials Science

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I will present our recent results on a novel approach to accelerate first-principles computational predictions of activated reactive processes at heterogeneous interfaces by exploiting Machine-Learning (ML) and conformal techniques. In our Conformal Sampling of Catalytic Processes (CSCP) approach, we combine stochastic sampling of activated mechanisms with ML force-fields in the form of message-passing Neural Network Potential (NNP), coupled with conformal transfer of databases to exploit information from existing data. We use methanol decomposition (of practical interest as hydrogen production process) as a proof-of-principle of double-ended search. Starting from fully worked-out Pt-based systems, we construct conformal databases that are exported to other systems to quickly derive a first-generation MACE (Multi-Atomic Cluster Expansion) NNP. The so-derived NNP is then improved with only 2 steps of active learning, leading to accurate DFT-accuracy-level predictions (errors on energy barriers of ≈0.03 eV), successfully including cases exhibiting surface diffusion, changes in adsorption sites and even change of catalytic sites as tests of catalytic path modifications. The approach is first demonstrated by exporting CH3OH-decomposition reaction paths from Pt(111) and Pt(100) to 7 other diverse metal catalyst (111) and (100) facets: Au, Pd, Ag, Cu, Ni, Co, Fe [1]. Then, in the case of the Cu-Pd system we show that equally good results are obtained for bimetallic alloy catalysts [2]. Finally, we demonstrate the successful extension of the approach to other catalytic processes, such as CO_2 reduction via hydrogenation. A way is thus open to efficient, high-throughput catalyst screening.

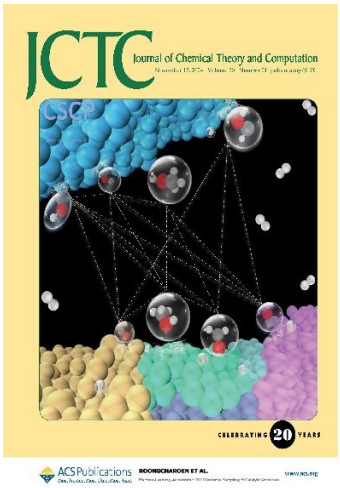

Fig. 1: A pictorial description of the CSCP approach.

References

[1] T. Roongcharoen, G. Conter, L. Sementa, G. Melani, and A. Fortunelli. *Machine-Learning-Accelerated DFT Conformal Sampling of Catalytic Processes*. J. Chem. Theory Comput. 20, 9580-9591 (2024).
[2] T. Roongcharoen, G. Conter, L. Sementa, G. Melani, and A. Fortunelli. Under review (2025).

[P2.33] Automated Workflows and Machine Learning models for X-ray spectra simulations: applications to Li-ion battery materials

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In the framework of material science, core-level spectroscopies are established strategies to probe the electronic structure and chemical environment of materials. While these techniques provide valuable information, their interpretation in complex systems is not straightforward, emphasizing the importance of theoretical insights from ab-initio approaches. On the other hand, the time required for computing an X-ray spectrum increases with the number of non-equivalent atoms, becoming prohibitively expensive for complex amorphous materials. This drawback can be addressed by employing a surrogate model that combines the precision of ab initio methods with computational efficiency [1]. We trained a machine-learning (ML) model based on Kernel Ridge Regression (KRR) [2], using atom-density descriptors for predicting X-ray Photoelectron Spectroscopies (XPS), by using core-electron Binding Energies (BE) as the target quantity. A comprehensive automated AiiDA workflow [3], integrating first-principles XPS simulation with sample sub-selection via Farthest Point Sampling (FPS), was employed to generate the critical amount of data needed for the training process. The ML models were trained on a representative dataset comprising about 250 lithiated Si-based structures, previously obtained through ab initio molecular dynamics (MD), DeePMD and grand canonical Monte Carlo simulations [4]. Validation on a dataset of around 50 structures demonstrated an accuracy of 0.1 eV, aligning with typical XPS experimental resolution. We leveraged the model to construct a stoichiometry map to identify the LixSi phases that form at various potentials in Si-based anodes.

References

[1] F. M. Paruzzo, A. Hofstetter, F. Musil, S. De, M. Ceriotti, and L. Emsley. *Chemical shifts in molecular solids by machine learning.* Nat. Commun. 9, 4501 (2018).
[2] V. L. Deringer, A. P. Bartok, N. Bernstein, D. M. Wilkins, M. Ceriotti, and G. Csanyi. *Gaussian Process Regression for Materials and Molecules.* Chem. Rev. 121, 10073 (2021).
[3] P. N. O. Gillespie, M. A. Hernandez Bertran, X. Wang, G. Pizzi, E. Molinari, and D. Prezzi. *Automated Workflows for Core-Level Spectroscopy Simulation.* Preprint (2024).
[4] F. Fu, X. Wang, L. Zhang, Y. Yang, J. Chen, B. Xu, C. Ouyang, S. Xu, F. Z. Dai, W. E. *Unraveling the Atomic-scale Mechanism of Phase Transformations and Structural Evolutions during (de)Lithiation in Si Anodes.* Advanced Functional Materials, 33, 37 (2023).

[P2.34] A combined G_0W_0/BSE approach to characterize polaron photoexcitations in reduced rutile TiO_2

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In reduced TiO_2, electronic transitions arising from polaronic excess electrons in localized band-gap states (BGS) are known to influence both photoabsorption and the photocatalytic activity of TiO_2 in the visible spectrum. Density Functional Theory (DFT) has been widely used to investigate the electronic excited states involved in these $d \rightarrow d$ excitations [1,2] and the BGS energy relative to the conduction band minimum. However, the accuracy of DFT is inherently limited by its theoretical framework, as in principle it is exact for ground state properties but fails to account for many-body effects and for the interactions between photogenerated electron-hole pairs, i.e., excitons. This has highlighted the need to move beyond DFT to a many-body perturbation theory (MBPT) framework. In this poster, I will present how a combined G_0W_0 and Bethe-Salpeter Equation (BSE) approach provides a powerful first-principles framework to characterize optical excitations from BGS, as observed in 2PPE experiments on hydroxylated rutile TiO_2(110) surfaces [1, 3] and optical absorption measurements on bulk rutile $Ti_{1-x}Nb_xO_2$[4]. Using a BSE spectrum projection tool onto defect states—justified by the negligible coupling between defect-states and valence-band transitions—we identified distinct classes of configurations where polaronic excitations exhibit similar spectral fingerprints. Interestingly, the polarons behave as isolated quasi-particles, with no optical coupling between them, and their response is influenced by the local chemical environment. In hydroxylated TiO_2(110), high-energy peaks (≥ 3 eV) arise from both $t_{2g} \rightarrow t_{2g}$ and $t_{2g} \rightarrow e_g$ transitions, depending on the polaron symmetry and its localization within the slab. The high-energy *d*-states involved in these transitions are mainly localized along the Ti_{5c} surface atoms, highlighting significant implications for the photocatalytic properties of rutile TiO_2(110). In contrast, these high-energy excitations are absent in $Ti_{1-x}Nb_xO_2$ bulk, where the absorption intensity increases with Nb concentration [4], with potential implications for the design of novel photovoltaic devices.

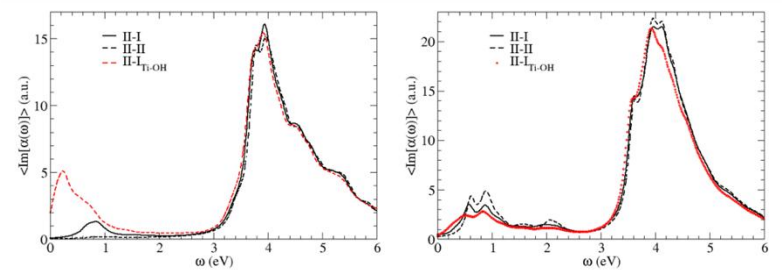

Fig. 1: averaged BSE absorption spectra for different polaronic configurations in TiO_2(110) with field along [1-10] (left) and [001] (right) crystallographic axes: (i) II-I, polarons in layers I and II; (ii) II-II just layer II.

References

[1] Z. Wang, et al. J. Am. Chem. Soc. 137, 9146 (2015).
[2] A. Tanner, et al. Phys. Rev. B 103, L121402 (2021).
[3] T. Wang, et al. J. Phys. Chem. Lett. 12, 10515 (2021).
[4] G. Sahasrabudhe, et al., Chem. Mater. 28, 3630 (2016).

[P2.35] Thermodynamics of chloride binding in trimeric coiled coils by molecular simulations

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Coiled coils, superhelical structures formed by two or more interwinding α-helices, are ubiquitous structural motifs in proteins, playing diverse roles in cellular signalling, gene regulation, and structural scaffolding [1]. Trimeric coiled coils recur in a diverse array of proteins, including viral fusion proteins (e.g., hemagglutinin of influenza, HIV envelope protein, and coronavirus spike protein), transcription factors (e.g., GCN4), and cytoskeletal proteins (e.g., laminins). Notably, the X-ray structures of certain trimeric coiled coils show central chloride ions, coordinated by symmetrically arranged asparagine residues (Fig. 1. To investigate the thermodynamics of halide binding to this site, we employ molecular simulations, using metadynamics and free-energy perturbation, both enhanced with replica exchange, to calculate the binding free energy (ΔG_B). Our results reveal that, despite the nearly identical local coordination of the ion, the calculated ΔG_B strongly depends on the overall protein structure. In particular, one short trimeric coiled coil, previously shown to be unstable in the absence of Cl^- by spectroscopic analyses [1], exhibits unfavorable binding of Cl^- ($\Delta G_B>0$). We discuss the origins of this result considering potential limitations of additive force fields, by employing QM/MM simulations for comparison. Furthermore, we designed a single-chain analog of the coiled coil that hosts the same Cl^- binding site, providing a tool to further investigate the relationship between halide binding and structural stability in these superhelices motives.

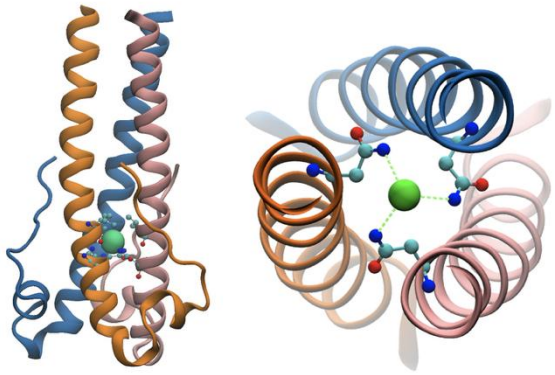

Fig. 1: Trimeric coiled coil of retrovirus envelop domain (PDB code: 1mof) in cartoon representation. Each monomer is shown with a different color, and the coordinated chloride ion is shown as a green sphere. The binding site is zoomed in on the right.

References

[1] D. N. Woolfson. *Understanding a protein fold: The physics, chemistry, and biology of α-helical coiled coils*. *J Biol Chem* 299, 4 (2023).

[2] M.D. Hartmann, O. Ridderbusch, K. Zeth, R. Albrecht, O. Testa, D. N. Woolfson, G. Sauer, S. Dunin-Horkawicz, A. N. Lupas, and B. Hernandez Alvarez. *A coiled-coil motif that sequesters ions to the hydrophobic core. Proc Natl Acad Sci USA* 106, 16950–16955 (2009).

[P2.36] Exciton-Phonon interaction from first principles in the theoretical spectroscopy of low-dimensional materials

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The problem of exciton-phonon interaction in crystals concerns the simultaneous description of the coupling of excited electron-hole pairs both within themselves and with lattice vibrations. It has become increasingly relevant to both experimental and theoretical research. It is invoked, for example, to explain fine structures in optical absorption and luminescence spectra of low-dimensional semiconductors, to model the width of excitonic spectral peaks, and to explain the out-of-equilibrium carrier dynamics in ultrafast spectroscopy.

I will discuss our recent progress in the modelling of exciton-phonon interaction in solids from first-principles using many-body perturbation theory [1], as well as its efficient implementation in the Yambo software package [2] as a combination of the state-of-the-art frameworks of the Bethe-Salpeter equation (describing excitons) and Density Functional Perturbation Theory (describing lattice vibrations).

I will then present two relevant applications. The first is concerned with the phonon-assisted luminescence of boron nitride in the hexagonal (AA') and rhombohedral (ABC) stackings. We show that we can quantitatively reproduce the experimental spectra and that the difference in the fine structures between the two systems are related to the exciton-phonon scattering selection rules. [3] The second application is about the lifetimes of the spin-orbit-split "A" and "B" bright excitons in monolayer MoS2. Here, the two excitonic states are in contact with different phonon-mediated scattering channels, resulting in a distinct behavior of their temperature-dependent linewidths, intensity renormalization factors, and dynamics. [4]

I will conclude with perspectives on the new possibilities opened by the quantitative knowledge of the interaction between optical excitations and lattice vibrations, namely the first-principles simulations of out-of-equilibrium, real-time excited-state dynamics in low-dimensional materials.

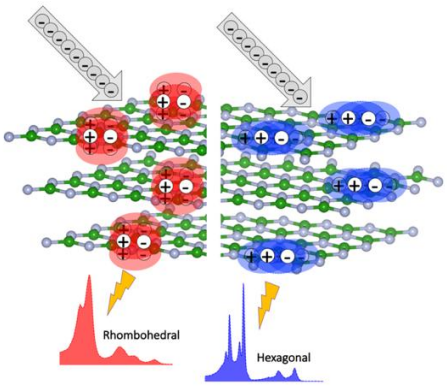

Fig. 1: Schematic representation of exciton-phonon spectroscopy in layered materials in the case of phonon-assisted cathodoluminescence: an electron beam generates excitons in the system, which later radiatively recombine thanks to the mediation of lattice vibrations. The fine structure of the luminescence spectrum depends on the symmetry of the crystal dictating the exciton-phonon selection rules.

References

[1] F. Paleari and A. Marini. Phys. Rev. B 106, 125403 (2022).

[2] D. Sangalli, et al. J. Phys. Condens. Matter 31, 32 (2019).

[3] M. Zanfrognini, et al. Phys. Rev. Lett. 131, 206902 (2023).

[4] F. Paleari, M. D'Alessandro, D. Varsano, and D. Sangalli. In preparation (2025).

[P2.37] Phosphorene as a Novel Two-Dimensional Nanomaterial: Studies of its Antimicrobial and Antiviral Properties

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Nanomaterials have recently attracted considerable attention for therapeutic applications against viruses and bacteria, offering promising alternatives to traditional treatments, such as antibiotics. Among various nanomaterials, phosphorene (BP) nanoparticles are particularly noteworthy for their unique properties, including light absorption and singlet oxygen generation, which are exploitable for photothermal and photodynamic antibacterial therapies [1–2].

In this study, a multiscale computational strategy, combining ab initio quantum mechanics, classical molecular dynamics, and Brownian dynamics simulations, was employed to investigate the interactions between BP nanoparticles and viral/bacterial biomolecules.

As a viral model system, domain III of the West Nile virus (WNV) E protein was selected for initial docking analyses, which identified possible adsorption orientations of the protein on phosphorene. These configurations were subsequently refined through multiple atomistic MD simulations in explicit solvent to improve conformational sampling and assess structural stability and folding behaviour.

Additionally, Lennard-Jones parameters for phosphorene within the OPLS force field were validated by comparing GROMACS molecular dynamics results with DFT-based results obtained by VASP, leading to parameter refinements to correct for underestimated interactions with amino acids.

In parallel, the study also explores the antimicrobial activity of BP nanoparticles through their interaction with bacterial membranes, aiming to elucidate the underlying mechanisms of action in relation to different lipid compositions.

The study aims to show how the project also investigates how the shape, size and surface conjugation of phosphorene with photosensitizers, influence membrane interactions, translocation rates and photokilling effects. The study aims to show how the project also investigates how the shape, size, and surface conjugation of phosphorene with photosensitizers, influence membrane interactions, translocation rates and photokilling effects. Furthermore, we examined the specific interactions between the nanoparticles and distinct molecular components of the membranes, providing insights into their potential as antimicrobial agents.

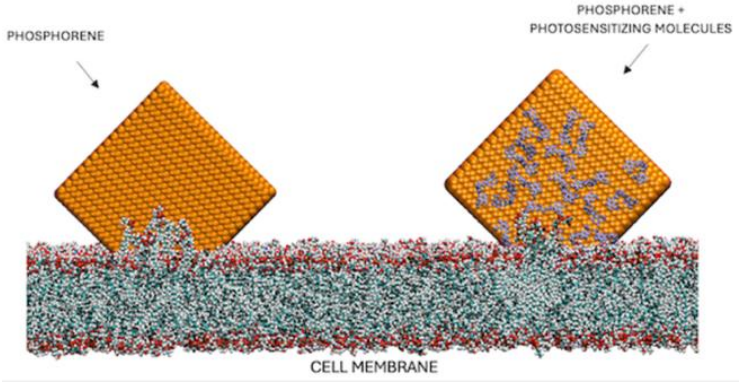

Fig. 1: The figure shows the two models considered for the study of the interaction between phosphorene nanosheets and bacterial membranes. The figure on the left shows the naked phosphorene penetrating the lipid bilayer, while the figure on the right illustrates a phosphorene nanosheet functionalized with a photosensitizing molecule, curcumin.

References

[1] Davis, Ryan, et al. *2D Layered Nanomaterials for Therapeutics Delivery. Current Opinion in Biomedical Engineering.* vol. 20 (2021).

[2] C. Caponio, et al. *Cyrene- and Water-Based Exfoliation of Black Phosphorus for Potential Nanolayer-Mediated Disaggregation of Insulin Fibrils*. FlatChem, vol. 45, (2024).

[P2.38] Electric control of spin and valley polarization in two-dimensional altermagnets

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Altermagnets are a special class of antiferromagnets where a zero net magnetization is enforced by symmetries that relate spin-up and spin-down sublattices but that, at the same time, allow for a finite spin splitting between energy bands, even in the absence of spin-orbit coupling. Despite this spin splitting, the presence of sublattice-relating symmetries requires band extrema –and thus valleys– in semiconducting altermagnets to be spin degenerate, although they might occur at different locations in the Brillouin zone for opposite spins. An external electric field can break these symmetries and thus give rise to a finite and controllable spin (and valley) polarization. This is particularly promising in two-dimensional (2D) materials where it is easy to apply a vertical electric field in a double-gate field- effect setup, provided that 2D altermagnets with suitable crystal symmetries are found. Here, by using first-principles simulations, not only we put forward an interesting family of 2D altermagnets that display the correct symmetries, but we also show the electric field effect is sizable in these materials and reaches the requirements needed for applications in spin-valleytronics.

Project
PRIN2022 project SECSY supported by Ministero Italiano dell'Università e della Ricerca.

[P2.39] Ab-Initio Investigation of the Aqueous Nafion-Platinum Interface for Enhanced PEM Fuel Cell Performance

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Proton exchange membrane fuel cells (PEMFCs) are among the most promising technologies for clean energy applications, relying on platinum (Pt) as the primary catalyst. The interaction between Nafion, the widely used polymer electrolyte, and Pt at the electrode interface plays a crucial role in the performance and durability of these fuel cells. While previous studies have focused on the macroscopic properties of Nafion, a detailed atomistic understanding of its interaction with Pt, particularly in the presence of water, remains incomplete. The interfacial behavior, proton transport, and electronic structure modifications induced by the electrolyte environment require further exploration through ab-initio methods [1-3].
In this study, we employ density functional theory (DFT) calculations to investigate the structural, electronic, and chemical properties of the Nafion-Pt interface in an aqueous environment. Our model incorporates explicit water molecules to simulate the solvation effects, providing a more realistic representation of the interface. We analyze charge transfer, adsorption energies, and electronic structure changes induced by hydration. Furthermore, charge density difference (CDD) analysis and projected density of states (DOS) calculations reveal key insights into the interaction between the polymer's sulfonic acid groups and the metal surface [4-6].
Our findings indicate that the presence of water significantly modifies the interfacial properties, enhancing the proton-conducting ability while altering the electronic states of Pt. The results contribute to a deeper understanding of catalyst degradation mechanisms and may guide future improvements in PEMFC performance through optimized electrode-electrolyte interfaces.

References

[1] J. H. Wee. *Applications of proton exchange membrane fuel cell systems*. Renewable and sustainable energy reviews 11(8), 1720-1738 (2007).
[2] S. J. Peighambardoust, S. Rowshanzamir, and M. Amjadi. *Review of the proton exchange membranes for fuel cell applications*. International journal of hydrogen energy 35(17), 9349-9384 (2010).
[3] K. Jiao, J. Xuan, Q. Du, Z. Bao, B. Xie, B. Wang, and M. D. Guiver. *Designing the next generation of proton-exchange membrane fuel cells*. Nature 595(7867), 361-369 (2021).
[4] R. J. Needs, M. J. Godfrey, and M. Mansfield. *Theory of surface stress and surface reconstruction*. Surface Science 242(1-3), 215-221 (1991).
[5] A. Tekin and B. Hartke. *Global geometry optimization of small silicon clusters with empirical potentials and at the DFT level*. Physical Chemistry Chemical Physics 6(3), 503-509 (2004).
[6] M. Capdevila-Cortada, Z. Łodziana, and N. López. *Performance of DFT+ U approaches in the study of catalytic materials*. ACS Catalysis 6(12), 8370-8379 (2016).

[P2.40] Self-healing polymers as alternatives for enhancing the stability of Li-ion batteries: molecular modeling studies

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Self-healing refers to the capability of a material to restore functionality after damage, and polymers with such characteristics are a valuable alternative to enhance the life cycle, efficiency, and safety of electronic and energy storage devices. In this work, we investigated the properties of a boronic acid- functionalized polyaniline - polyvinyl alcohol (B@Pani-PVA) binder as an alternative to increasing the life cycle of Li-ion batteries. This binder combines Pani's intrinsic conductivity and flexibility with boronic acid's ability to interact with the OH groups of PVA and form hydrogen bonds, thus enhancing the self-healing behavior [1]. We combined different methodologies to understand the role of functionalization, the influence of the size chain, and the structural properties of B@Pani-PVA. From density functional theory calculations, we gained insights into the structural modifications induced by the presence of the boronic acid radical and its interaction with the amine group. We showed that this interaction played a key role in determining the oligomer chain growth pattern and stability [2]. We also employed Bader's atom-in-molecule (AIM) analysis to investigate the number, kind, and strength of the long-range intra-molecular and inter-chain interactions (mainly hydrogen bonds and van der Waals) and found a clear correlation with the length and conformation of the oligomers. From classical molecular dynamics simulations, we obtained properties such as density, radial distribution function, self-diffusion, and hydrogen bond formation. These insights provide a solid foundation for the rational design of advanced PANI-based materials with tailored properties for energy storage and self-repair applications.

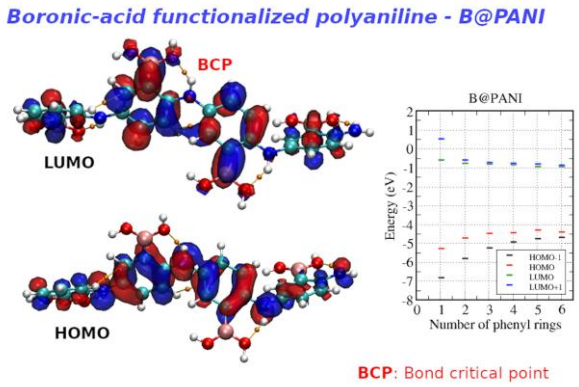

Fig. 1: Frontier orbitals of 4-B@Pani oligomer, and variation in HOMO-LUMO energies as a function of oligomer chain size.

References

[1] R. Maji, M.A. Salvador, A. Ruini, R. Magri, and E. Degoli. *A first-principles study of self-healing binders for next-generation Si-based lithium-ion batteries.* Materials Today Chemistry 29, 101474 (2023).

[2] A. K. Mishra and P. Tandon. *A Comparative Ab Initio and DFT Study of Polyaniline Leucoemeraldine Base and Its Oligomers.* J. Phys. Chem. B 113, 14629-14639 (2009).

[P2.41] Envelope-function theory of inhomogeneous strain for hole-spin qubits in silicon and germanium

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Strain is a common feature of semiconductor nanostructures, arising from the lattice mismatch between heterogeneous layers and the cooling down of materials with different thermal-expansion coefficients [1,2]. It significantly alters the system properties, representing either a problem (if uncontrolled) or a resource, e.g., to enhance the carrier mobility [3]. Inhomogeneous-strain engineering can be used to efficiently improve Rabi frequencies and g-tensors in Si spin qubits [4]. However, the rigorous inclusion of strain within the k-dot-p formalism – the reference framework for the simulation of charge carriers in semiconductors – has been so far limited to the homogeneous case, which is accounted for by the theory of Bir and Pikus [5].

In our work [6], we have developed a complete theory to include inhomogeneous strain in the k-dot-p framework, by generalizing the Bir-Pikus approach via concepts from differential geometry. We obtained an envelope-function Hamiltonian that is applicable to a variety of semiconductor systems. It includes several new terms, which depend on the spatial derivatives of the strain tensor and could not be deduced from previous approaches. I will discuss the implications of our findings for the simulation and strain engineering of hole-spin qubits in Si and Ge quantum dots.

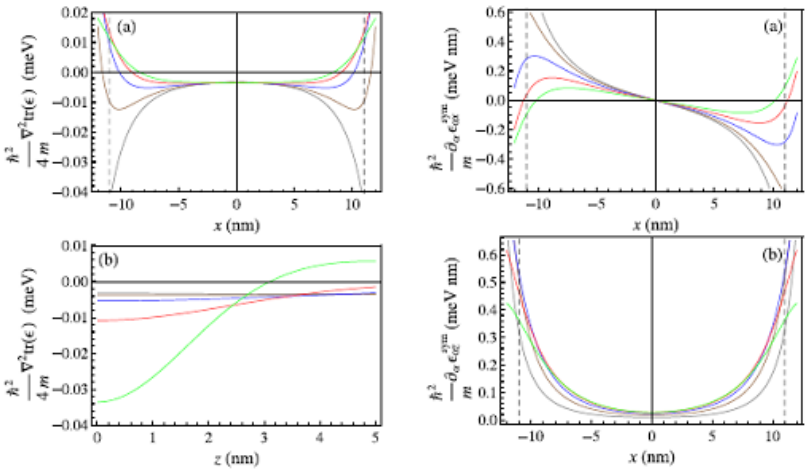

Fig. 1: Some of the new Hamiltonian terms, depending on the spatial derivatives of the strain tensor.

References

[1] J. J. Pla et al. *Strain-induced spin-resonance shifts in silicon devices.* Phys. Rev. Appl. 9, 044014 (2018).

[2] Y. Sun, S. E. Thompson, and T. Nishida. *Physics of strain effects in semiconductors and metal-oxide-semiconductor field-effect transistors.* J. Appl. Phys. 101, 104503 (2007).

[3] Y.-M. Niquet, C. Delerue, and C. Krzeminski. *Effects of strain on the carrier mobility in silicon nanowires.* Nano Lett. 12, 3545 (2012).

[4] J. C. Abadillo-Uriel, E. A. Rodríguez-Mena, B. Martinez, and Y.-M. Niquet. *Hole-spin driving by strain-induced spin-orbit interactions.* Phys. Rev. Lett. 131, 097002 (2023).

[5] G. Bir and G. Pikus. *Symmetry and Strain-induced Effects in Semiconductors.* Wiley, New York (1974).

[6] A. Secchi and F. Troiani. *Envelope-function theory of inhomogeneous strain in semiconductor nanostructures.* Phys. Rev. B 110, 045420 (2024).

[P2.42] Accurate Treatment of Metallic Screening in Many-Body Calculations from First Principles

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Many-Body Perturbation Theory calculations in the GW approximation have proven to be a reliable scheme for the computation of quasiparticle (QP) band structures of materials [1]. In metallic systems, QP corrections are generally smaller than in semiconductors, but still necessary to properly describe spectroscopic properties [2], especially at low dimensionality.

GW is a computationally expensive method, especially in metals that require an accurate description in both frequency and k-space. Typically, the long-wavelength limit of intraband transitions is treated by adding a Drude term at the plasmon energy [3]. However, the ab-initio determination of the plasmon energy is demanding and the Drude method is a too simplistic approach for certain metals and semimetals [4]. Here, we present an efficient method for computing the screened potential of metals, evaluated through a Monte Carlo integration combined with interpolation techniques [5,6]. This method was first developed for 2D semiconductors, where it led to a dramatic speed-up of the otherwise slow k-point convergence [7]. We generalize its usage by developing proper interpolation techniques for 3D and 2D metals. In this way, it is possible to capture the effect of intraband transitions without the need for additional parameters and reproduce the QP band structure with reduced k-point grids.

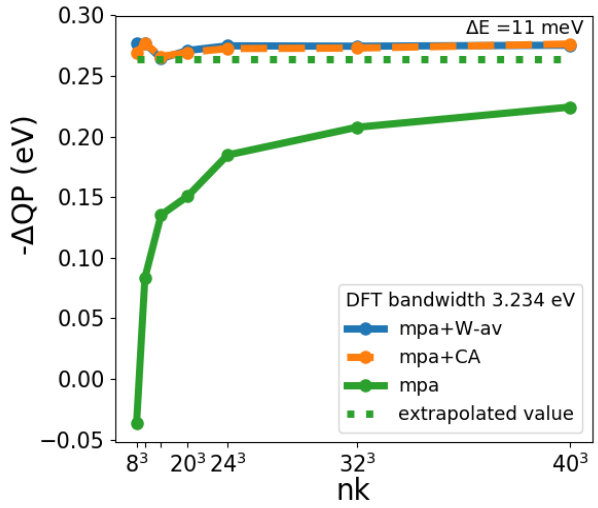

Fig. 1: QP correction to the bandwidth of a 3D metal bulk Na with respect to the number of points in the k-grid, computed with (blue line) and without (green line) the W-av method.

References

[1] G. Onida, et al. Rev. Mod. Phys. 74, 601 (2002).
[2] M. Cazzaniga, et al. Phys. Rev. B 82, 035104 (2010).
[3] K. H. Lee and K. J. Chang. Phys. Rev. B 49, 2362 (1994).
[4] D. A Leon, et al. Phys. Rev. B 107, 155130 (2023).
[5] F. H. da Jornada, et al. Phys. Rev. B 95, 035109 (2017).
[6] W. Xia, et al. npj Comput. Mater. 6, 118 (2020).
[7] A. Guandalini, et al. npj Comput. Mater. 9, 44 (2023).
[8] T. Chiarotti, et al. Phys Rev R. 4, 013242 (2022).

[P2.43] Green's function methods towards the exascale

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Materials are crucial to science and technology and connected to major societal challenges ranging from energy and environment, to information, communication, and manufacturing. The accuracy and efficiency of electronic-structure methods are driving a new paradigm in research. With simulations becoming increasingly faster and efficient, they serve as indispensable tools for understanding, predicting, and designing material properties. Many-body perturbation theory (MBPT) and Green's function methods offer an accurate description of excited electrons. However, these approaches come with significant computational cost. Conventional GW implementations have a computational cost that scales as $O(N^4)$ with respect to the system size N, limiting the scope of GW calculations.

The efficiency of electronic-structure calculations depends both on the development of computational algorithms and hardware technology. Here we present new algorithm developments recently implemented in the Yambo code [1,2], aiming at improving accuracy and efficiency, such as the W-av method [3] and the multi-pole approximation (MPA) [4,5] as well as a new python software layer (Yambopy) able to perform post-processing operations and manage Yambo workflows.

In the effort of improving hardware performance, solutions based only on many-cores architectures are being conspicuously replaced by heterogeneous or accelerated architectures. We will discuss the strategy devised for the GPU porting of the Yambo code, as well as the resulting speedup of the calculations. Yambo is now able to efficiently run on all presently available accelerated machines in Europe, alternatively adopting CUDA-Fortran, OpenACC, and OpenMP offloading programming models.

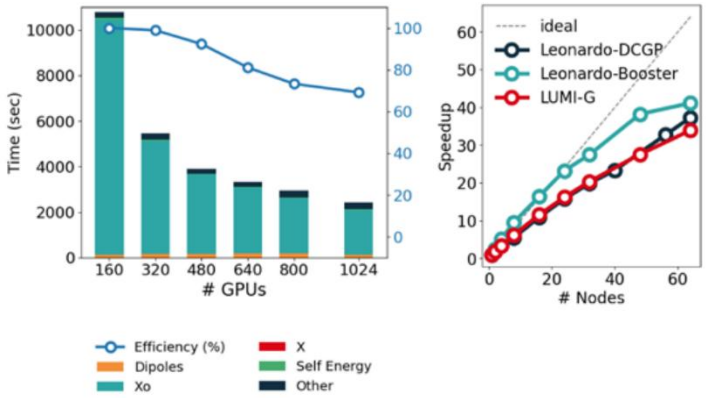

Fig. 1: Calculation of quasi-particle corrections on a graphene/Co interface. On the left, the scalability test on Leonardo-Booster (CINECA), while at the right a speedup comparison between Leonardo-DCGP, Leonardo-Booster and LUMI-G (CSC) for the same system but with reduced parameters.

References

[1] D. Sangalli, et al. *Many-body perturbation theory calculations using the yambo code.* Journal of Physics: Condensed Matter 31, 325902 (2019).

[2] A. Marini, C. Hogan, M. Gruning, and D. Varsano. *Yambo: An ab initio tool for excited state calculations.* Computer Physics Communications 180, 1392 (2009).

[3] A. Guandalini, P. D'Amico, A. Ferretti, and D. Varsano. *Efficient GW calculations in two-dimensional materials through a stochastic integration of the screened potential.* npj Computational Materials 9, 44 (2023).

[4] A. Guandalini, et al. *Efficient calculations via interpolation of the screened interaction in momentum and frequency space: The case of graphene.* Phys. Rev. B 109, 075120 (2024).

[5] D. A. Leon, A. Ferretti, D. Varsano, E. Molinari, and C. Cardoso. *Efficient full frequency GW for metals using a multipole approach for the dielectric screening.* Phys. Rev. B 107, 155130 (2023).

[P2.44] The structure-function relation in disordered amorphous materials

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The concept of disorder is not only related to structural factors, but also to the functional properties of the systems [1]. The understanding of disorder in amorphous materials widely employed in industrial applications and daily life is the key to control their mechanical, electrical, and chemical properties [2,3], but it is far from being understood. Here, we consider two classes of disordered materials, namely chalcogenide glasses and amorphous metal oxides.

Chalcogenide glasses are gaining recognition as a valuable class of materials for both optical and electronic devices, in view of their ability to rapidly switch between amorphous and crystalline phases or between high- and low-conductive states by controlling temperature or current. In particular, we consider the case of doped GeSe alloys, which gained pride of place because of their tailorable electrical properties in Ovonic Threshold Switching (OTS) applications. By using a unique multi-functional approach that combines molecular dynamics simulations, thermodynamics, machine learning and statistical analysis [1,4,5]. We investigate the complex interplay between composition and doping on the structural and thermal properties of GeSe alloys.

Amorphous metal oxides are employed in a wide range of applications. In particular, the interface between crystalline-HfO_2 and amorphous-Al_2O_3 show promising results for memristive devices. However, defects such as oxygen vacancies significantly alter their properties. Despite in crystals the vacancy formation requires the simple removal of an atom, in amorphous the choice of which atom should be removed is much more complex due to the different chemical environment. We studied the O-vacancy formation at glass-crystalline interfaces defining what is a vacancy in an amorphous material from a structural and electronical point of view, finding that amorphous intrinsically contains vacancies that can be employed to tune the electrical response of the material.

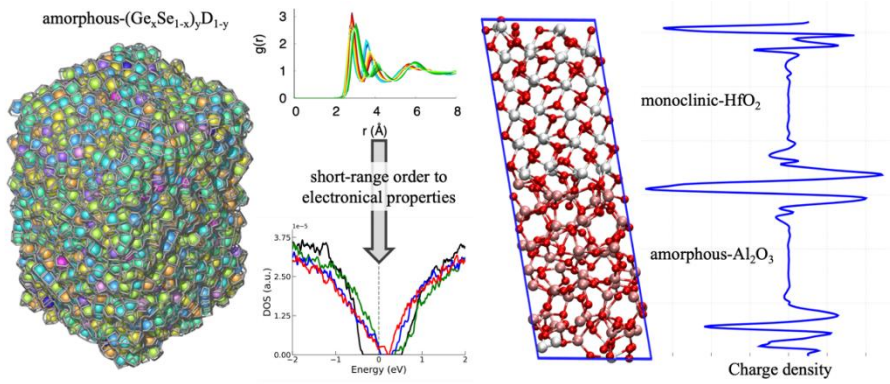

Fig. 1: From left to right: the amorphous structure of doped-GeSe systems colored accordingly to its Voronoi geometry; the radial distribution functions and Density of States; the interface between m-HfO_2/a-Al_2O_3 and the charge density across the interface.

References

[1] F. Tavanti and A. Calzolari. Acta Mater 266, 119676 (2024).
[2] A. Slassi, et al. Adv. Electron. Mater. 9 (4), 2201224 (2023).
[3] A. Slassi, et al. Appl. Surf. Sci. 689, 162455 (2025).
[4] F. Tavanti and A. Calzolari. ACS Omega 7 (27), 23255–23264 (2022).
[5] F. Tavanti, B. Dianat, A. Catellani, and A. Calzolari. ACS Appl. Electron. Mater. 2 (9), 2961–2969 (2020).

[P2.45] Computer modeling across energy scales: Tritiated graphene for neutrinos studies

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Neutrinos studies are often based on their nuclear interaction with ^{3}H (tritium, T) and on the analysis of the energy spectrum of the subsequently emitted β electron. In particular, the international PTOLEMY collaboration [1] aims primarily at improving the upper limits of the neutrino mass, by analysing the continuum spectrum of the β released upon decay of T in He, and secondarily to detect the discrete spectrum of the β emitted upon capture of the cosmologic "relic" neutrinos, produced just after the Big Bang. Tritiated graphene is the chosen as active material, since its capability of loading it in almost 1:1 stoichiometry with C promises an unpreceded concentration of T and the consequent possibility of increasing the resolution of measurements. In addition, the solid-state form allows a better control of the emitted β radiation, while the large exposed surface prevents spoiling the energy spectrum. However, using a solid substrate also bears disadvantages [2]. The electronic, dynamical, and chemical properties of the material are modulated by the loading level and distribution of T. This influences the β spectrum in several ways, especially in its end point, which bears the most relevant information on neutrino mass.

For this reason, we have started a series of interdisciplinary studies [3] combining computational and modelling methods typical of high and low energy physics. Here we report the evaluation of T/He binding energy as a function of loading level and distribution (Fig. 1), before and after the T decay, performed with unconventional declinations of Density Functional Theory [4], which explores non adiabatic dynamics. We use these potentials to evaluate the decay rate in different conditions, which involves a fully quantum treatment of the nuclear coordinates. We subsequently follow the fate of He and the signals produced in the substrate after its escape from it on different time scales. These studies unravel the solid-state effects on the β spectrum and will be used to improve the accuracy of the measurements. As side results, we observe specific vibrational and electronic signals generated post-reaction on the substrate, which propagate information on the nuclear reaction over the graphene sheet by means of charge and spin density waves.

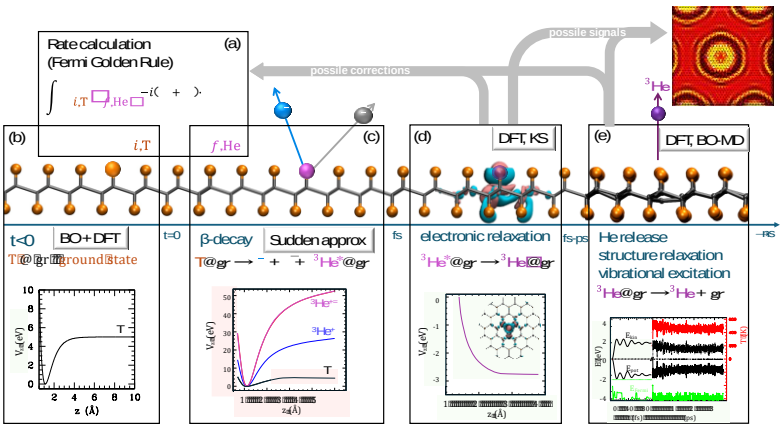

Fig. 1: Modeling of the reaction T →He + e + ν, with T on graphene (a) Scheme of calculation of the decay rate, with ψ the wave functions of T and He just after and before decay. (b) State of T@graphene before decay. The T-gr interaction potential is reported. (c) State of He@graphene just before decay. In the very early instants after decay, the electronic structure of the system corresponds to the ground state with T before decay, which is an excited state with respect to the new system with He. The extraction potentials for the He ions in these conditions are reported. (d) System after the electronic relaxation to the new ground state evaluated with DFT within the Kohn-Sham scheme: electrons move towards He to compensate the additional nuclear charge and the potential becomes repulsive. (e) fs to ps time scales Born-Oppenheimer molecular dynamics of the system. He is released and the recoil excites specific modes of the substrate. Vibrational dynamics can be used to add further correction to the rate evaluation. Vibrations can also be associated to charge density waves (structure on the top right corner) and spin density waves.

References

[1] M. G. Betti, et al. *Neutrino physics with the PTOLEMY project: active neutrino properties and the light sterile case.* JCAP 07, 047 (2019).

[2] A Apponi, et al. *Heisenberg's uncertainty principle in the PTOLEMY project: A theory update.* Physical Review D 106, 053002 (2022).

[3] G. Menichetti, A. Casale, A. Esposito and V. Tozzini. *Computer modeling across energy scales: Tritiated graphene for neutrinos investigation.* Submitted.

[4] A. Casale, A. Esposito, G. Menichetti, and V. Tozzini. *Solid state effects on β-decay spectra: a multi-methodological study of tritiated graphene*. In preparation.

[P2.46] Elucidating K adsorption and intercalation in Gr/MoS_2 heterostructures

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Van der Waals heterostructures (vdWHs) enable an unprecedented combination of extraordinary properties in few-atom-thick layers and are expected to foster the development of myriad applications in many fields, including electronics, photo- and optoelectronics, sensing, and catalysis. In energy storage, their electronic and structural diversity can introduce a fine modulation of heterointerfaces, able to effectively enhance intercalation of foreign species and to provide promising alternatives to graphitic anodes for post-Li technologies [1].

With the aim of elucidating interfacial properties and processes taking place at the level of individual atomic layers, we investigate potassium adsorption and intercalation in few-layer MoS_2 and MoS_2/Gr interfaces. We explore the effect of K concentration and adsorption sites on the structural, thermodynamic, and electronic properties of single-layer MoS_2, and discuss the differences with respect to the case of few-layer MoS_2 and MoS_2/Gr heterostructure, as well as the case of few-layer Gr alone [2]. Furthermore, we investigate the modification of the phonon modes upon K adsorption for a few selected cases to track the H-to-T' transition between MoS_2 polymorphs.

Our results are compared with micro-ARPES, Raman and PL experiments performed by the group of Riccardo Frisenda and Carlo Mariani at the SMARTLab of University of Rome La Sapienza and the SOLEIL synchrotron (CNRS - CEA Paris-Saclay).

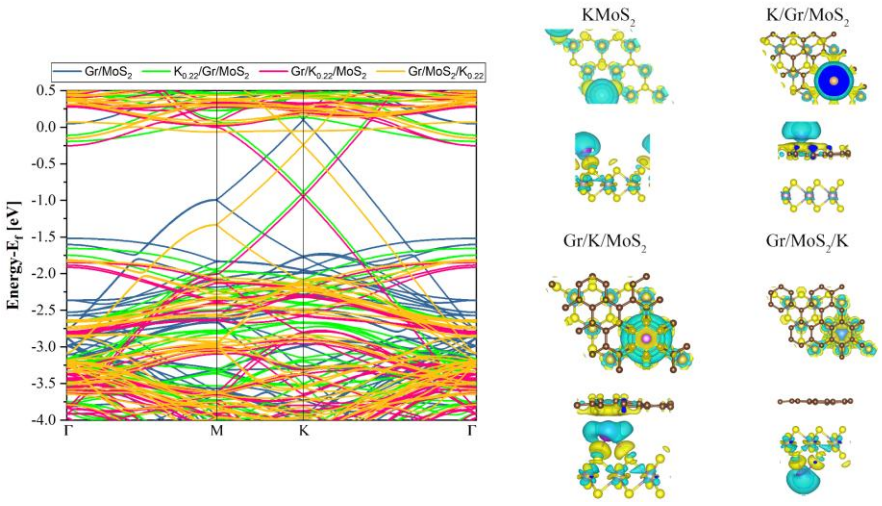

Fig. 1: Band structures and charge density difference plots (isosurface level: 0.0007e/Å3) of $KMOS_2$, K/Gr/MoS_2, Gr/K/MoS_2, and Gr/MoS_2/K.

References

[1] R. Zhang, et al. *How does Molybdenum Disulfide Store Charge: A Minireview.* ChemSusChem 13, 1354 (2020).

[2] D. Marchiani, N. Jimenez Arevalo, M. Sbroscia, C. Cardoso, D. Prezzi, C. Mariani, M. G. Betti, and R. Frisenda. Preprint (2025).

Project

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[P2.47] Coherent Vibrations Promote Charge-Transfer across a Graphene-Based Interface

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Understanding the impact of nuclear motion on the efficiency and timing of charge transfer (CT) at the donor–acceptor interface is crucial for designing high-performance optoelectronic devices. In collaboration with experimental partners, we investigate the CT dynamics in a cobalt phthalocyanine–graphene (CoPc–Gr) [1]. Experimentally, photocurrent detection in coherent multidimensional spectroscopy is used to excite a donor CoPc and collect the charge transferred to a 2D acceptor Gr layer. The CoPc–Gr interface exhibits an ultrafast electron-transfer signal that presents an oscillating time evolution modulated by coherent vibrations originating from the laser-excited CoPc states.

Using time-dependent density functional theory with an optimally tuned range-separated hybrid functional, we characterize the excited energy landscape of the CoPc–Gr system and correlate it with the Fourier analysis of the beatings appearing in experimental data and the Raman features. Our analysis reveals two key states: a low-oscillator-strength bright state with orbitals purely localized on CoPc and a CT character state exhibiting significant π–π coupling between CoPc and Gr. Through per-mode reorganization energy analysis [2], we identify specific molecular vibrations that dynamically couple these states, facilitating CT at the interface.

The combination of theoretical and experimental tools offers a deeper understanding of how nuclear coherence influences interfacial CT, providing fundamental design principles for next-generation optoelectronic devices.

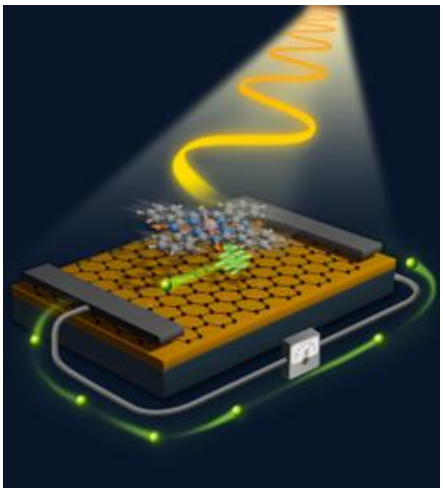

Fig. 1: Coherent Vibrations Promote Charge-Transfer across a CoPc–Gr Interface

References

[1] A. Casotto, P. S. Rukin, E. Fresch, D. Prezzi, S. Freddi, L. Sangaletti, C. A. Rozzi, E. Collini, and S. Pagliara. *Coherent Vibrations Promote Charge-Transfer across a Graphene-Based Interface.* Journal of the American Chemical Society 146, 14989 (2024).

[2] P. S. Rukin, D. Prezzi, and C. A. Rozzi. *Excited-State Normal-Mode Analysis: The Case of Porphyrins.* J. Chem. Phys, 159 (24), 244103 (2023).

[P2.48] Computational Insights into Organic Halide Perovskite Solar Devices Incorporating Electroactive Interlayers

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Inverted perovskite solar cells (PSCs) have emerged as a promising alternative to conventional structures, offering advantages such as simplified fabrication and improved stability. However, commonly used electron transport layers (ETLs) in p-i-n devices, such as fullerene-based materials, suffer from stability issues and induce a highly defective perovskite/ETL interface, featuring trap-mediated non-radiative recombination, which adversely impacts both the efficiency and stability of the resulting solar cells. The introduction of organic spacer moieties at the perovskite/ETL with stabilization effects has been proposed as an effective strategy to mitigate surface-assisted recombination and increase the stability of the device. However, conventional molecular passivators are electronically insulating, resulting in charge confinement with respect to the light-absorbing material, thus limiting their functionality. In this context, optimizing the electronic properties of the passivating layer material offers a promising approach to overcome performance limitations by enhancing charge transport to the ETL.

In this contribution, we present the results of an experimental and theoretical study concerning the introduction of electroactive spacer moieties at the interface between the perovskite absorber and fullerene-based ETLs in inverted PSCs. We employ *ab-initio* molecular dynamics and Density Functional Theory to elucidate the experimental findings and to unveil the underlying mechanisms connected to the interfacial charge transfer and improved stability brought about by the electroactive spacers. The use of electroactive spacers as ETL in fullerene-free devices is also explored.

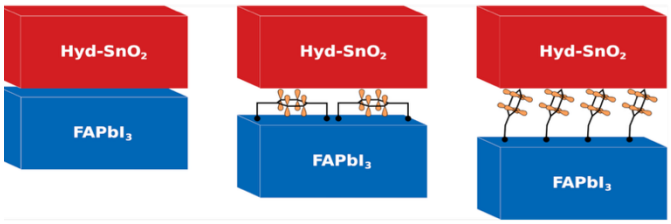

Fig. 1: Schematic picture of the studied fullerene-free solar cell device based on FAPbI3/Hyd-SnO2 stacking. Organic molecular spaces are introduced at the interface between the perovskite photoabsorber and the electron transport layer. Suitably chosen molecular interlayers can act as defect passivators as well as charge transfer facilitators due to their electroactive nature, leading to improved operational stabilities and power conversion efficiencies of the perovskite solar cell device.

References

[1] G. AlSabeh, et al. *Aryl-Acetylene Layered Hybrid Perovskites in Photovoltaics.* Angew. Chem. Int. Ed. 2025, e202417432 (2025).

[2] L. Li, M. Wei, V. Carnevali, H. Zeng, M. Zeng, R. Liu, N. Lempesis, F. T. Eickemeyer, L. Luo, L. Agosta, M. Dankl, S. M. Zakeeruddin, U. Roethlisberger, M. Grätzel, Y. Rong, and X. Li. *Buried-Interface Engineering Enables Efficient and 1960-Hour ISOS-L-2I Stable Inverted Perovskite Solar Cells*. Adv. Mater. 36, 2303869 (2024).

[3] J. Jeong, T. Chawanpunyawat, M. Kim, V. Sláma, N. Lempesis, L. Agosta, V. Carnevali, Q. Zhang, F. T. Eickemeyer, L. Pfeifer, Y. Kim, J. W. Song, H. Lu, M. Almalki, S.-I. Mo, S. M. Zakeerudin, U. Rothlisberger, D. S. Kim, P. J. Dyson, and M. Grätzel. *Carbazole Treated Waterproof Perovskite Films with Improved Solar Cell Performance*. Adv. Energy Mater. 15, 2401965 (2025).

[4] V. Carnevali, L. Agosta, V. Slama, N. Lempesis, A. Vezzosi, A., and U. Rothlisberger. *Nano-size nature of the α-FAPbI $ _3 $ by means of large-scale ab initio simulations*. Preprint, arXiv:2409.04219 (2024).

[P2.49] Optimizing Aptamer-Gold Interfaces for Enhanced Detection of West Nile Virus

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In this work, we combined a multiscale computational strategy with Surface Plasmon Resonance (SPR) experiments to investigate how DNA aptamers interact with gold surfaces when targeting the envelope protein of the West Nile Virus (WNV). This integrative approach aims to support the design of biosensors with heightened sensitivity, addressing the urgent need for reliable diagnostics for WNV, which currently lacks specific treatments.

Although DNA aptamers hold great potential in biosensing applications, their immobilization on solid supports often diminishes their binding capabilities. We explored the influence of surface morphology by comparing two gold nanoclusters, Au144(SR)60 and Au314(SR)96 (SR = thiolate ligand), with a flat Au(111) surface, to determine optimal anchoring configurations. Furthermore, we assessed how physiological conditions, particularly high ionic strength environments, affect both nanocluster stability and aptamer-protein binding efficiency.

Our findings offer valuable insights into aptamer functionalization on gold nanoparticles (AuNPs), providing a robust platform for engineering more effective biosensors. This methodology not only supports improved detection of WNV but can also be adapted for diagnostics targeting a wide array of viral pathogens.

[P2.50] Magnetic Properties of Dysprosium (Dy) Single-Atom Magnets in ZnO Substrates

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We aim to unravel site-dependent magnetic properties of dysprosium (Dy) atoms embedded in ZnO substrates by means of an all-electron DFT analysis employing linearized augmented plane wave (LAPW) methodology with LDA+U and hybrid functionals, using the Wien2K code. This work follows a series of previous investigations on rare-earth (RE) adatoms on $SrTiO_3$ [1], BaO [2]and ZnO surfaces [3] and delves into the possibility to anchor the RE atoms within the oxide matrix while maintaining the single-atom magnet character, which is the main goal of the ongoing PRIN2022 “MAGNETISE” project.
Our electronic structure calculations elucidate where the Dy atoms are preferentially found in the ZnO matrix, in the bulk or near Zn-polar or O-polar terminated surfaces, and the role of O and Zn defects. Relevant parameters (Bader charges, crystal field parameters) are extracted to assist the interpretation of XMCD spectra of Dy-doped ZnO films recently acquired at the SOLEIL synchrotron radiation source.

References

[1] V. Bellini, S. Rusponi, J. Kolorenč, S. K. Mahatha, M.A. Valbuena, L. Persichetti, M. Pivetta, B. V. Sorokin, D. Merk, S. Reynaud, D. Sblendorio, S. Stepanow, C. Nistor, P. Gargiani, D. Betto, A. Mugarza, P. Gambardella, H. Brune, C. Carbone, and A. Barla. *Slow Magnetic Relaxation of Dy Adatoms with In-Plane Magnetic Anisotropy on a Two-Dimensional Electron Gas*, ACS Nano 16, 11182 (2022).
[2] B. V. Sorokin, M. Pivetta, V. Bellini, D. Merk, S. Reynaud, A. Barla, H. Brune, and S. Rusponi. *The Impact of Lattice Distortions on the Magnetic Stability of Single Atoms: Dy and Ho on BaO(100)*, Adv. Funct. Mater. 2213951 (2023).
[3] In preparation [2025].

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Day 1: Thursday June 05, 2025

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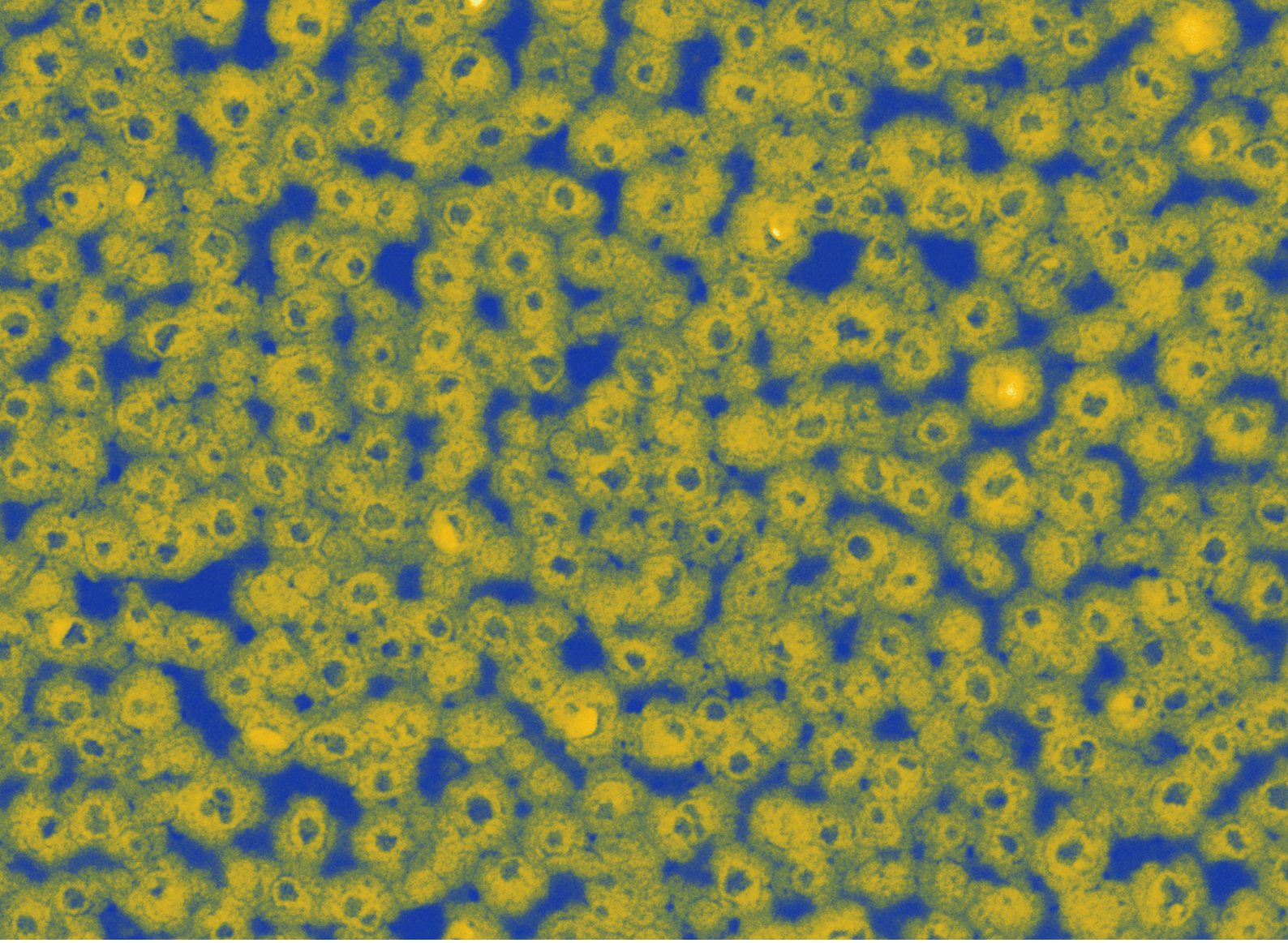

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