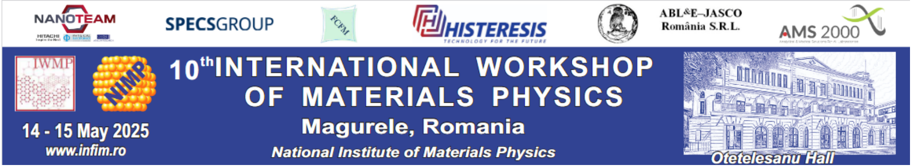
THE MISSION



The National Institute of Materials Physics (NIMP) proudly announces the organization of the 10th edition of the International Workshop of Materials Physics (IWMP).

The aim of the workshop is to highlight recent applications of advanced theoretical and computational methods for materials science. Recent results obtained with state-of-the-art computational (DFT, molecular dynamics, machine learning, finite element, *etc*.) and theoretical methods are encouraged presentation subjects.

The workshop is organized as a 2-day event, from May 14 to 15, 2025, and will feature invited talks and poster sessions only. By bringing together experts from various fields of computational materials science we aim to promote the exchange of information and open new avenues for collaborations, projects, or mutual training stages for early-career researchers.

THE VENUE

The Oteteleșanu Hall in Măgurele has a storied past dating back to the 19th century (1843), when it was built by the influential Oteteleșanu family. Initially serving as their private residence, it underwent a significant transformation in 1894, becoming the esteemed “Ioan Oteteleșanu Institute for Girls” under the auspices of the Romanian Academy.

Across its existence, the Otetelesanu Hall has stood witness to the dynamic evolution of Romanian history, from periods of subjugation at the cross-roads of three Empires to the victorious pursuit of independence and modernization. During its journey, the hall has endured three major wars, the vicissitudes of Communism, and the arduous path back to Democracy, navigating through cycles of transformation, neglect, and revitalization. Through it all, the Oteteleșanu Hall has remained a steadfast symbol of resilience amidst political turmoil and societal shifts.

Following a decade of careful restoration overseen by NIMP, Oteteleșanu Hall has been rejuvenated as the headquarters of the Culture and Physics Foundation in Măgurele, the International Centre for Advanced Training and Research in Physics (CIFRA), and the DRIFMAT cluster.

Today, it serves as a prestigious venue for international events like IWMP, embodying both its historical scope and contemporary relevance while upholding its unwavering, 130-years-old commitment to education and scientific advancement.

In the present day, the Oteteleșanu Hall stands as a testament to the cultural legacy of Măgurele, offering a captivating window into the past while remaining an integral part of the local community vibrant present.

THE HOST

NATIONAL INSTITUTE OF MATERIALS PHYSICS

Established in 1949, the Institute of Physics of the Romanian Academy was founded by Horia Hulubei, a distinguished scientist renowned for his ground-breaking contributions to various fields of physics, including Raman, X-rays, Compton, atomic, and nuclear physics. Hulubei earned his PhD in Paris under the tutelage of Nobel Prize laureates Pierre Curie and Maria Skłodowska-Curie.

In 1956, the Institute underwent a division resulting in the formation of two separate entities: the Institute of Atomic Physics (IFA) in Măgurele & the Bucharest Institute of Physics (IFB), the latter led by the Acad. Prof. Eugen Bădărău. E. Bădărău, a prominent professor from Sankt Petersburg and Cernăuți Universities, played a pivotal role in advancing the Romanian school of physics, particularly in the study of electrical discharges in gases and plasma.

Relocating to Măgurele in 1974, the Institute experienced further transformation in 1977 with the amalgamation of laboratories from IFB and IFA, forming the Institute of Physics and Technology of Materials. In 1996 it was officially rebranded the National Institute of Materials Physics (NIMP) following a national accreditation process, subsequently re-accredited in 2008 and 2016. Throughout its history, NIMP has been home to distinguished physicists such as Acad. Eugen Bădărău, Acad. Radu Grigorovici, Acad. Ioan Iovitz Popescu, Acad. Margareta Giurgea, Acad. Rodica Mănăila, or Acad. Vladimir Țopa.

Over the past fifty years, NIMP has emerged as a leading research institution in Romania, investing over 35 million EUR in a new laboratory building equipped with state-of-the-art research facilities and the restoration of the historic Oteteleșanu Hall. Internationally, NIMP has played a significant role as one of the founders of the Central European Research Infrastructure (C-ERIC) and as an associated member of the Francophone University Agency (AUF). Additionally, it hosts a UNESCO category 2 centre – the Centre for Advanced Training and Research in Physics (CIFRA).

THE PROGRAM

of the 10th edition of the International Workshop of Materials Physics

14 May, 2025

INVITED TALKS

08:15	**Registration – *Oteteleșanu Hall***
08:45	**Official opening – Lucian PINTILIE, Scientific Director of NIMP**
Session 1: Chairman – Lucian PINTILIE	
9:00	**Jorge INIGUEZ** Luxembourg Institute of Science and Technology, LUXEMBOURG **Hafnia ferroelectrics: A singular challenge for theory and simulation**
9:40	**Sergiu CLIMA** IMEC, Leuwen, BELGIUM **First-principles screening for OTS/SOM chalcogenide materials**
10:20	**Santanu SAHA** University of Limoges and Institut de Recherche sur les Céramiques (IRCER), Limoges, FRANCE **Adapting physico-chemical affinities in first principles design of new materials**
11:00	**Coffee break**
11:15	**Adolfo O. FUMEGA** Academy of Finland, Aalto University, FINLAND **Computational modeling of emergent phases in moiré materials**
11:55	**Andrei BERNEVIG** Princeton University, USA **Moiré systems as quantum simulators of strongly correlated Hamiltonians**
12:35	**Lunch**
Session 2: Chairman – Marius Adrian HUȘANU	
14:00	**Bilal TANATAR** Department of Physics, Bilkent University, Ankara, TURKEY **Studies of localization within Aubry-André model**
14:40	**Krzysztof WOHLFELD** Institute of Theoretical Physics of the Faculty of Physics of the University of Warsaw, POLAND **Altermagnetism from a strong-coupling perspective**
15:20	**Jan MINAR** New Technologies Research Center (NTC), University of West Bohemia, Pilsen, CZECHIA **Quantum materials and magnetic phenomena studied by spin-resolved ARPES: Theoretical perspectives**
16:00	**Coffee break**
16:15	**Andrei MANOLESCU** Reykjavik University, ICELAND

	Magnetic-flux periodicity in core/shell semiconductor/superconductor nanowires
16:55	**Cătălin PASCU MOCA** University of Oradea, ROMANIA **Kondo compensation and quantum criticality in superconducting and fractionalized systems**
17:35	**Poster Sessions**
18:30	**Dinner**

15 May, 2025

INVITED TALKS

Session 3: Chairman – Alin VELEA	
9:00	**Stephan ROCHE** ICREA Institució Catalana de Recerca i Estudis Avancats, Barcelona, SPAIN **Linear scaling quantum simulation methodologies**
9:40	**Marius STAN** University of Chicago, USA **Artificial intelligence for material design**
10:20	**Alin M. ELENA** Scientific Computing Department, Science and Technology Facilities Council, Daresbury Laboratory, Daresbury, UK **Machine learned interatomic potentials for modelling porous materials**
11:00	**Coffee break**
11:15	**Felix MOCANU** Department of Materials, University of Oxford, Oxford, UK **Computational design of high energy density cathode materials for Li-ion batteries**
11:55	**Larisa VON RIEWEL** Excelitas (former Heraeus) Noblelight, Bayern, GERMANY **Microscopic investigation of the slurry drying process and binder migration in Li-ion battery anodes using computational chemistry**
12:35	**Lunch**
Session 4: Chairman – Cristian Mihail TEODORESCU	
14:00	**Claudiu GENES** Max Planck Institute, Erlangen, GERMANY **Quantum optics with atoms and molecules: Analytical approaches**
14:40	**Vidar GUDMUNDSSON** Science Institute, University of Iceland, ICELAND **Arrays of quantum dots or rings in a FIR-photon cavity**
15:20	**Coffee break**
15:35	**Krzystof WIECZERZAK** Department of Materials Science, Faculty of Mechanical Engineering and Aeronautics, Rzeszow University of Technology, Rzeszow, POLAND *ONLINE PRESENTATION*

	Exploring CuAgZr metallic glasses for biomedical use: A study using combinatorial synthesis, high-throughput experiments, and machine learning
16:15	**George Alexandru NEMNES** Faculty of Physics, University of Bucharest, ROMANIA **Hybrid perovskite materials: From perovskite solar cells to memristive elements**
17:30	**Poster Sessions**
18:00	**Conference Dinner**

Abstracts
of
Invited Talks

INVITED TALK

Hafnia ferroelectrics: A singular challenge for theory and simulation

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CMOS-compatible hafnia ferroelectrics hold great promise for the development of nano-devices that take advantage of their permanent and switchable electric polarization, which has made them a focus of attention. But that is not all: surprisingly, these materials are proving to constitute a ferroelectric class of their own, displaying many intrinsic behaviors that seem genuinely unprecedented and certainly lay outside the "standard model" of soft-mode ferroelectricity in perovskite oxides. In this talk I will present first-principles results to discuss and explain some of those intriguing intrinsic properties. I will focus on the piezoelectric response of hafnia ferroelectrics [1,2], which – by comparison with the (trivial) behavior of ferroelectric perovskites – will allow me to illustrate some of their most puzzling features: for example, the unconventional (and yet to be understood) nature of ferroelectric switching in these materials. I will also summarize other recent theory simulation works in my group, addressing the stabilization of the ferroelectric polymorph in hafnia-based superlattices [3] and the induction of structural softness and large electromechanical responses [4], respectively. As we will see, when it comes to hafnia, wherever we look we tend to find surprising results that contradict our expectations and question our understanding. I will conclude with a personal outlook for simulation work in the field, briefly commenting on challenges and opportunities.

Work funded by the Luxembourg National Research Fund (FNR), as of late through grant INTER/NWO/20/15079143/TRICOLOR. Projects done with B. Mukharjee, S. Dutta, N.S. Fedorova and H. Aramberri (LIST), as well as many other collaborators, *e.g.*, A. Gruverman's group (NebraskaLincoln), C. Dubourdieu's group (Helmholtz-Zentrum Berlin), *etc*.

References:

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INVITED TALK

First-principles screening for OTS/SOM chalcogenide materials

Sergiu CLIMA*, Daisuke MATSUBAYASHI, Fabian DUCRY, Taras RAVSHER, Daniele GARBIN, Attilio BELMONTE, Geoffrey POURTOIS
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To find environment-friendly Ovonic Threshold Switching (OTS [1]) materials, we performed a systematic material screening for As/Se-free ternary compositions by using firstand second- principles calculations [2]. OTS materials are sought for two-terminal selectors, needed to suppress the sneak-path leakage currents (Fig. 1) [3–5] but can also be used as stand-alone selector-only memory (SOM) [6,7]. By using DFT-computed Born effective charges, we observed that it is feasible to predict material OTS behavior (with the so-called OTS gauge Fig. 2) [2,8,9]. Focusing on ternary compounds (comprising 14 elements Fig. 3) and using several screening filters (material thermal stability, semiconducting electronic properties), we down-selected from more than 13000 to ~1400 compositions, for which we generated amorphous models and computed the DFT electronic structure: mobility gaps and trap gaps for 10 models per composition for statistical averaging of computed properties. For a smaller subset of compositions that are thermodynamically stable with open electronic gap (Fig. 4), we computed the OTS gauge (Fig. 2). Additionally, the machine-learning derived spinodal temperature of the promising compositions was used to exclude the compositions unstable against de-mixing (potentially resulting in reliability issues). As a result, we identified more than a dozen of promising compositions for stand-alone OTS memory or RRAM selector applications.

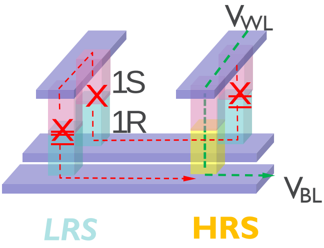

Fig. 1: SELECTOR cuts the parasitic materials. leakage on half-biased LRS cells, while allowing the correct reading of HRS cell.

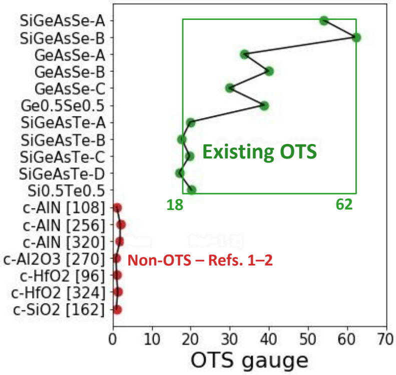

Fig. 2: DFT-computed OTS gauge for experimentally-known OTS is an order of magnitude higher than for non-OTS materials.

	B	C	N	~~O~~
	Al	Si	P	S
Zn	Ga	Ge	~~As~~	~~Se~~
~~Cd~~	In	Sn	Sb	Te

Fig 3: Elements that were considered for OTS materials.

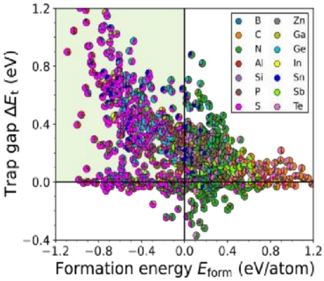

Fig.4: Only open electronic gap and stable compositions were considered.

Further understanding of the SOM mechanism is required. Using the DFT and Non-Equilibrium Green-Functions (NEGF) approaches, we investigate the feasibility of few possible mechanisms at the device/ atomic level (atomic segregation and field-sensitive local traps), however the results are far from conclusive and further work is required.

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NOTES

INVITED TALK

Adapting physico-chemical affinities in first principles design of new materials

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Design of new functional materials has been traditionally driven by rigorous experimental investigations often guided by notion of chemical bonding. Due to the nature of the work, the processes are resource intensive and time consuming and thereby strongly limiting large scale exploration over different plausible candidates [1]. In addition, ab-initio methods have been used posteriori to provide atomic-scale description of different emerging properties.

However, in the last two decades there has been a paradigm shift in the usage of *ab initio* based methods as an *a posteriori* approach towards accelerating the searches and identifying potential compounds. Primarily, (*i*) crystal structure prediction [2] and (*ii*) high throughput screening [3] has become state of the art methods. While crystal structure methods efficiently explores the potential energy surface of a given composition to identify local minima (phase space), high-throughput screening explores the possibility of realizing a composition on a given structural template (chemical space) [4]. In brief, one method is focused on exploration of phase space and other chemical space. These methods has been applied successfully for exploration of wide class of materials [5]. But, their adaptation for efficient exploration of multinary system is challenging with strong rise is complexity and computational cost.

A possible enroute towards addressing these challenges is to first identify the preferred atomic arrangements (local minima in phase space) and adapting recurring structural templates for exploration over different chemically alike species/compositions. In the talk, I will provide brief introduction to these methods, their limitations and our recent works on (i) binary hydrides for room temperature superconductors [6] and (ii) family of organic chalcogenide-halide perovskites as new photovoltaic materials [7–8].

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INVITED TALK

Computational modeling of emergent phases in moiré materials

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Layered van der Waals materials are one of the most promising platforms for engineering emergent phases in condensed matter physics. The weak van der Waals bonding between their layers allows to easily reach the single-layer limit, offering intrinsic degrees of freedom to artificially design new materials. In particular, moiré patterns can arise due to the lattice mismatch between two or more van der Waals layers stacked together, leading to several coexisting length scales. These can naturally occur when two layers of different van der Waals materials with distinct lattice parameters are stacked together, or when layers of the same material are twisted or strained. The interplay between the different length scales can promote exotic phases of matter. Due to the large number of atoms involved in the description of moiré materials, new computational methodologies need to be developed to theoretically study their emergent phases.

In the first part of this talk, we will discuss how to model twisted spin-spiral van der Waals multiferroics [1]. Spin spiral multiferroics are materials that display simultaneously a spin spiral magnetic order and ferroelectricity, showing a strong magnetoelectric coupling. This can be exploited to control the magnetic order using electric fields. Here, we will uncover the different topological skyrmion phases that can arise in twisted spin spiral multiferroics. We will see that these skyrmion phases are originated by the interplay between the spin spiral and the moiré length scales. We will show how these topological magnetic textures can be tuned with external electric fields due to the magnetoelectric coupling displayed by these multiferroics.

In the second part of this talk, we will analyze a novel methodology to study correlated states in super-moiré materials [2]. This class of materials arise when three or more different layers are stacked together creating a moiré modulation on top of a moiré material. Therefore, the moiré pattern itself will feature a long-range modulation, giving rise to a super-moiré pattern. Modeling super-moiré materials requires solving systems with millions of atoms and incorporating electronic interactions in a self-consistent manner, a task challenging beyond current atomistic electronic structure methods. We will demonstrate a technique that combines a kernel polynomial method with a quantics tensor cross interpolation with matrix product states. This methodology is capable of solving interacting electronic models in real space for systems with millions of atoms, allowing us to compute interaction-induced symmetry-broken states in those systems while treating interactions in a self-consistent manner.

References:

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INVITED TALK

Moiré Systems as quantum simulators of strongly correlated Hamiltonians

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We will review the beginning of experimental and theoretical studies of moiré systems and their evolution up to present. We will show how thousands of p orbitals in a moiré unit cell of graphene can create single Heavy fermion at moiré scale, and how the interaction between such fermions can lead to a quantum simulator of an Anderson model. We will then present a catalogue of possible twistable materials and show how a huge variety of strongly interacting models can be realized in twisted homo and hetero twisted bilayers and multilayers of these materials.

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INVITED TALK

Studies of localization within Aubry-André model

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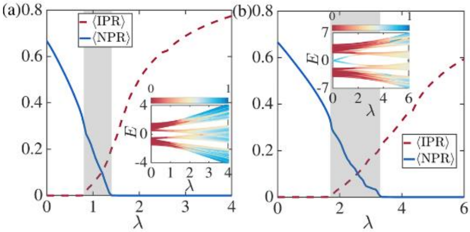
We begin by introducing an analysis of the single particle localization phenomenon in a quasiperiodic lattice in one-dimension [1]. Giving a detailed derivation of the Aubry-André Hamiltonian we describe the localization transition through the analysis of stationary and dynamical observables. In particular, the stationary properties investigated are the inverse participation ratio, the normalized participation ratio and the energy spectrum as a function of the disorder strength. Two dynamical quantities allow us to discern the localization phenomenon, being the spreading of an initially localized state and the evolution of population imbalance in even and odd sites across the lattice. This basic model is useful in the understanding of localization phenomena, a topic of current interest in fields of condensed matter, ultracold atoms and complex systems.

We next consider a recent application [2]. We consider a one-dimensional dimerized lattice with staggered quasiperiodic disorder, and show that after the localization transition, some of the localized eigenstates become extended for a range of intermediate disorder strengths. Eventually, the system undergoes a second localization transition at a higher disorder strength, leading to all states being localized. We also show that the two localization transitions are associated with the mobility regions hosting the single-particle mobility edges. We establish this reentrant localization transition by analyzing the eigenspectra, participation ratios, and the density of states of the system.



The inverse participation ration (IPR) (red dashed curve) and normalized participation ration (NPR) (blue solid curve) are plotted as a function of λ for (a) $\delta = 0.5$ and (b) $\delta = 3$ for a system of size $L = 13530$. The shaded regions indicate the critical or the intermediate regimes. The color maps in the insets show the plots of IPR associated to all eigenmodes E with respect to λ for values of δ of the main figure.

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INVITED TALK

Altermagnetism from a strong-coupling perspective

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Recently, a new form of magnetism has been proposed – so-called altermagnetism. While altermagnetism has mostly been discussed within the itinerant picture, here I would like to provide a brief overview of three important aspects related to altermagnetism in the strong-coupling limit. First, I will discuss how to search for materials that should show altermagnetic properties in the strong coupling limit [1,2]. Next, I will explore whether there is a way to observe altermagnetism in strongly correlated copper oxides – *i.e.*, the parent compounds to high-temperature superconductors [3]. Last but not least, I will show that strongly coupled altermagnets should show spin-momentum dependent quasiparticle damping in ARPES [4,5].

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INVITED TALK

Quantum materials and magnetic phenomena studied by spin-resolved ARPES: Theoretical perspectives

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Quantum materials exhibit a complex interplay between electronic correlations, topology, and magnetism, placing them at the forefront of condensed matter physics and quantum technology. Understanding these systems requires disentangling spin-orbit coupling, electron-electron interactions, and magnetic fluctuations under realistic conditions, including finite temperatures and structural disorder. Spin- and time-resolved angle-resolved photoemission spectroscopy (STARPES) is a crucial technique for probing electronic and spin structures in magnetic and topological materials. However, quantitative interpretation of spin-ARPES data necessitates advanced theoretical models that accurately capture electronic states, spin textures, and dynamic responses to external fields.

I will present a theoretical framework based on the fully relativistic multiple-scattering Green function KKR method [1], effectively modeling spin-dependent photoemission. This approach includes correlation effects via dynamical mean-field theory (DMFT) [2] and describes spin fluctuations using the alloy analogy model [3]. I will also discuss advances in calculating light-induced electronic excitations [4], highlighting their relevance to spin-ARPES studies of topological and magnetic quantum materials.

A novel application is the one-step model of photoemission in studying altermagnets and kagome magnetic materials. Altermagnets, exhibiting unconventional time-reversal symmetry breaking without net magnetization, are explored in RuO2 and MnTe [5,6]. Spin-ARPES combined with the one-step model provides insights into lifted Kramers spin degeneracy, revealing their potential for spintronics. In kagome magnetic materials, persistent flat band splitting and selective band renormalization are observed in FeSn thin films [7], highlighting unique correlation effects and topological phenomena. These developments offer a comprehensive framework for exploring magnetic phenomena and spin dynamics in complex quantum materials.

Acknowledgements
I would like to thank the Quantum Materials for Sustainable Technologies (QM4ST) project with Reg. No. CZ.02.01.01/00/22_008/0004572, cofunded by the ERDF as part of the MŠMT.

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INVITED TALK

Magnetic-flux periodicity in core/shell semiconductor/superconductor nanowires

Andrei MANOLESCU
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Core/shell nanowires are radial heterostructures consisting of a central nanowire core surrounded by a thin layer of a second material. Over the past two decades, semiconductor materials have been combined to create tubular conductors, where charge carriers are confined within the shell. These nanowires have a range of optical and electrical properties that make them attractive for various applications. In particular, in the presence of a magnetic field oriented along the nanowire, flux periodic oscillations of the conductance have been observed experimentally, with period h/e, corresponding to the Aharonov-Bohm effect.

In the recent years a layer of a superconductor metal has been added to such core/shell semiconductor nanowires. In this case, the superconductivity can penetrate the semiconductor material, a phenomenon called the proximity effect, leading to complex quantum phenomena such as Andreev or Majorana bound states with topological properties. The semiconductor shell becomes now a superconductor, where the charge carriers are supposed to have the effective mass of a semiconductor.

With a superconductor metal layer completely surrounding the nanowire, experimental investigations showed that, in the presence of an axial magnetic field, the charge current travelling along the proximitized semiconductor oscillates with period h/2e, like in a tubular metallic superconductor, corresponding to the Little-Parks effect. In other words, the charge unit is 2e instead of the e value as in the normal state of the semiconductor. In such experiments the critical supercurrent was measured by defining a narrow Josephson junction along the nanowires with a discontinuity of the metallic shell.

Surprisingly, with a superconductor metal layer covering only a half of the nanowire circumference, the critical Josephson current within the semiconductor shell still oscillates with period h/2e, indicating that the proximity effect acts such that the tubular semiconductor still becomes a full-shell superconductor. If so, a natural question arises: what is the minimal contact area between the superconductor metal and the semiconductor nanowire required to fully proximitize the semiconductor shell?

We model the device using a quantum mechanical approach based on the Bogoliubov-de Gennes Hamiltonian, where the superconductor is characterized by a gap parameter, and where a self-energy term is created at the interface with the semiconductor nanowire.

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INVITED TALK

Kondo compensation and quantum criticality in superconducting and fractionalized systems

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Magnetic impurities in superconductors give rise to rich quantum many-body phenomena, governed by the interplay between Kondo screening and superconducting pairing. In a conventional metal, an embedded impurity spin is screened by the Kondo effect, forming an extended correlation cloud. In an s-wave superconductor, however, the impurity gives rise to Yu-Shiba-Rusinov (YSR) states, and a quantum phase transition occurs between screened and unscreened phases when the superconducting gap Δ exceeds the Kondo temperature T_K. We show that the Kondo cloud persists in both phases, albeit with only partial screening in the unscreened regime. The concept of Kondo compensation is introduced as a universal measure of cloud integrity, directly related to the impurity's g-factor, which can be probed experimentally via bias spectroscopy.

Beyond conventional metals and superconductors, we investigate the impact of a pseudogap density of states, $\rho(\omega) \sim |\omega|^{\varepsilon}$, on Kondo screening. In the generic absence of particle-hole symmetry, increasing the exchange coupling j drives a quantum phase transition from a partially screened doublet state to a fully screened many-body ground state. At the critical coupling j_c, the Kondo compensation follows a scaling law, $\kappa(j<j_c) = 1 - g(j)$, with the local g-factor vanishing as $g \sim |j - j\_c|^{\beta}$. Combining perturbative drone fermion techniques with non-perturbative NRG computations, we determine the critical exponent $\beta(\varepsilon)$, revealing a non-monotonic dependence on ε. These results establish that the Kondo cloud forms continuously in the presence of a weak pseudogap as the phase transition is approached.

For a larger impurity spin $S=1$, partial screening leads to an underscreened Kondo effect, giving rise to an additional quantum phase transition between a partially screened doublet state and an unscreened triplet state as Δ/T_K increases. We demonstrate that the Kondo compensation exhibits a universal jump at this transition, vanishing deep in the unscreened phase while approaching 1/2 in the partially screened regime. Spin-spin correlation functions reveal an oscillatory behavior with a short-distance power-law decay and a long-distance exponential suppression governed by the superconducting correlation length ξ_Δ. These properties are further explored via spectral function calculations, employing numerical renormalization group (NRG) and density matrix renormalization group (DMRG) methods.

Finally, we extend these concepts to one-dimensional superconductors with fractionalized excitations. In such systems, conduction electrons split into gapless charge and gapped spin modes, with the impurity coupling exclusively to spin degrees of freedom. This interaction drives a local quantum phase transition and gives rise to the “fractionalized Shiba state.” The impurity-induced tunneling spectrum exhibits universal power-law scaling, with an exponent of -1/2 at half-filling due to gapless charge fluctuations forming a Luttinger liquid. At finite temperatures, spectral features remain universal at the critical point. These findings provide new insights into impurity physics in exotic superconducting environments.

Our results unify diverse aspects of Kondo screening, quantum phase transitions, and impurity physics in superconducting, and fractionalized systems, offering novel experimental signatures and theoretical insights into strongly correlated quantum matter.

NOTES

INVITED TALK

Linear scaling quantum simulation methodologies

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I will present efficient *linear scaling quantum simulation methodologies (www.lsquant.org)* which enable the simulation of realistic (three-dimensional) models of complex (disordered) matter [1] and recently extended to nonequilibrium regimes (hot electrons and energy dissipation) [2].

I will present the foundations of these approaches and illustrate them in various situations, such as spin transport properties in two-dimensional materials, topological insulators and van der Waals heterostructures, as well as in nonequilibrium equilibrium regimes when the transport physics is fundamentally altered by electronic population redistribution. We will review the power of these methodologies to lift interpretation ambiguities of experimental data, such as giant spin Hall effect in graphene-based devices proximitized graphene with strong spin-orbit coupling materials. The combination of bulk-like approaches (Kubo formalism) and multiterminal transport methods (as for instance implemented within Kwant) will be shown essential to explore topological effects in complex disordered materials, while novel forms of dynamical topological phenomena will be shown in regimes driven by light illumination and absorption.

Finally, the availability of smart scientific workflows will be introduced as gamechanger for accelerating the use of these techniques in academic and industrial floors [3].

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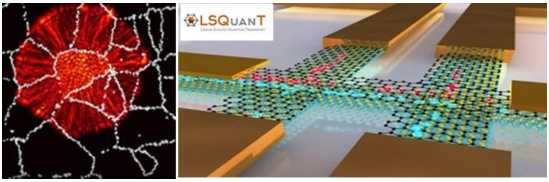

NOTES

INVITED TALK

Artificial intelligence for material design

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Understanding material properties and designing improved materials require the coupling of experimental and computational methods to create predictive models. Furthermore, comprehensive evaluations of data and model quality are necessary. With the volume, variety and rate of data generation continuously increasing, human analysis becomes extremely difficult, if not impossible. In this talk, elements of Artificial Intelligence such as machine learning and computer vision, are coupled with diffraction experiments and Bayesian statistics. The value of the approach is illustrated using the study of hafnia (HfO_2), a material used for computer memory.

Fig. 1 shows the methodology used to couple experiments and computations to understand and optimize HfO_2 properties. In step (1), HfO_2 samples are acoustically levitated, and x-ray and neutron diffraction measurements initialize the active learner. In step (2), an unsupervised machine-learning algorithm explores the phase space, screening for best atom configurations. In step (3), an iterative process that involves supervised machine learning optimizes the interatomic potential [1], [2].

The results show that the machine learning algorithm reduces the design time and effort by a factor of 10 – compared to quantum mechanical (Density Functional Theory) and classical (*Ab Initio* Molecular Dynamics) calculations – while maintaining accuracy. The intelligent program finds the optimal inter-atomic potential and crystal structure improving the material properties.

Furthermore, a discussion of current and future applications of AI demonstrates that the human-machine partnership can positively impact material science.

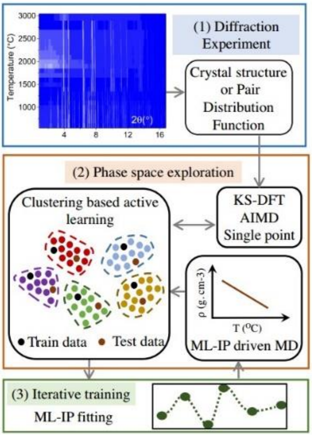

Fig. 1: Methodology employed to couple experiments and computations for understanding and optimizing HfO_2.

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NOTES

INVITED TALK

Machine learned interatomic potentials for modelling porous materials

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Zeolites and metal organic frameworks (MoFs) are two important classes of porous materials. Zeolites, naturally or synthetized crystalline aluminosilicates, are fundamental to a wide range of industrial applications owing to their diverse structural characteristics, thermodynamic and mechanical stability under varying conditions and due to their geological importance. Metal-organic frameworks, synthetic crystalline materials comprising of a metal node and an organic ligand, are highly porous and versatile materials studied extensively for applications such as carbon capture, water harvesting and treatment, catalysis, biological applications, batteries and sensors, However, modelling such materials is not without challenges, due to their size and the need for accuracy, for example in MOFs, computing phonon-mediated properties like thermal expansion and mechanical stability, remains challenging due to the large number of atoms per unit cell, making traditional Density Functional Theory (DFT) methods impractical for high-throughput screening. In this talk we will present various applications of machine learnt interatomic potentials to porous materials. We will present how MLIP foundation model can be employed to study zeolites [1,2] and how one can fine tune them to increase their accuracy in the case of MOFs [3]. We introduce a new model that can predict successfully phonons and thermal expansion and bulk moduli in agreement with DFT and experimental data for several well-known MOFs. These results highlight the potential of newly developed MACE-MP-MOF0 in guiding MOF design for applications in energy storage and thermoelectrics.

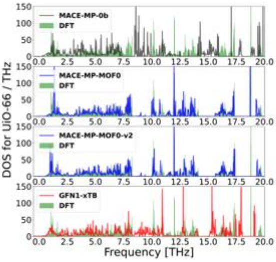

Fig.1: Density of states (DOS) in the frequency range (20 THz) for the investigated MOFs obtained with the linear tetrahedron method with a pitch of 0.01 THz predicted by the respective methods

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NOTES

INVITED TALK

Computational design of high energy density cathode materials for Li-ion batteries

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The electrification of transport is crucial for reducing carbon emissions and mitigating climate change. Improving battery performance, particularly cathode storage capacity, is essential for achieving long-range autonomy and reducing the cost of electric vehicles [1]. Li-rich materials, such as transition metal layered oxides, offer nearly double the capacity of stoichiometric counterparts by utilizing redox reactions on oxygen anions. However, they face significant challenges, including first-cycle hysteresis and voltage fade on subsequent cycles.

This lecture will explore the atomic origins of voltage and capacity fade in Li-rich cathode materials and discuss strategies to mitigate degradation [2]. By leveraging density functional theory (DFT) simulations, we can probe the connection between cathode electrochemistry and the material's electronic structure. DFT-calculated enthalpies help describe the thermodynamics of charging and to fit cluster expansion models which can be correlated with experimental measurements [3, 4]. Further analysis of electronic structure can provide atomistic insights into the redox mechanisms while dynamical simulations can probe the kinetics of structural transformations.

Additionally, machine-learning (ML) techniques are increasingly used to screen for new materials and extend the time and length scales of simulations while maintaining accuracy of quantum-mechanical approaches. The lecture will discuss the deployment and challenges of ML in the context of transition-metal oxides and cathode materials.

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NOTES

INVITED TALK

Microscopic investigation of the slurry drying process and binder migration in Li-ion battery anodes using computational chemistry

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Batteries play a crucial role in modern society, impacting various aspects of our daily lives and the wider economy. From renewable energy integration to electromobility and environmental impact, batteries are an integral part of the transition to a more sustainable and resilient energy system, supporting technological advances and improving quality of life.

Battery manufacturing typically involves three main stages: electrode manufacturing, cell assembly and formation, ageing and validation. The first stage, electrode manufacturing, remains the central part of the manufacturing chain and is subject to continuous development from a scientific and industrial perspective. New materials are being explored and developed to improve the electrochemical properties and robustness of next generations of batteries. Anode and cathode materials research is revisiting the roots of lithium-based electrodes and revealing how atomic structure, doping, electrolytes, binders and additives interact in manufacturing processes to influence the stability of coatings.

Slurry formulation and drying are the next critical steps in battery manufacturing, particularly for lithium and sodium-ion batteries. The slurry is a mixture of active materials, conductive additives, binders, and solvents, which is then coated onto metal foils to create the battery's electrodes. The slurry drying involves the removal of the solvent from the slurry-coated electrodes to leave a solid layer of active material, binder and conductive additives on the metal foil, which defines properties such as porosity, adhesion, conductivity, electrode film electrochemical characteristics and performance. Advanced drying techniques based on photonic mechanisms are investigated to achieve the desired electrode mechanical stability, and manufacturability. Advanced characterization techniques and modelling approaches based on computational physics and chemistry are often used to predict and optimize the properties of the slurry and the final electrode

This study employs computational chemistry based multiscale-simulation methods, including molecular dynamics (MD) and dissipative particle dynamics (DPD), to explore binder migration, active layer adhesion, and the role of binders at varying drying rates. Furthermore, IR spectra of the main components atomic structures were calculated using the NWChem plugin inside Simcenter Culgi. Initially, the structures were geometrically optimized with the Hartree-Fock (HF) *ab-initio* method using 6-31G* atomic orbitals basis set. Subsequently, the IR spectra were calculated alongside energy optimization using the same basis set. Results indicate good agreement with experimental findings, emphasizing the potential of this computational model to enhance battery formulations and process parameters in a cost-effective and sustainable manner at an early stage in the discovery process.

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NOTES

INVITED TALK

Quantum optics with atoms and molecules: analytical approaches

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Superradiance and subradiance are fundamental aspects of the open system dynamics of dense ensembles of quantum emitters exhibiting spontaneous emission rates well below or well above the rate for a single isolated system. At the purely theoretical level, superradiance has been first discussed by Dicke in 1954, in the context of accelerated decay of an ensemble of identical N initially inverted two-level quantum systems. In practice, such cooperative behavior associated with super- and subradiance at low excitation levels, has been observed in the 1930s by Jelley and Scheibe, in the context of molecular aggregates: unexpectedly large absorption cross-sections have been recorded for dye molecules. This has been later explained by Kasha in the 1960s as stemming from the alignment of the transition dipole moments of the many nanometer-spaced monomers forming the aggregate.

We analytically tackle such issues with methods of open quantum system dynamics, in particular quantum Langevin equations and master equations.

For the problem of Dicke superradiance we identify an exact analytical solution for the time evolution of the density operator, valid for any time t any number N of emitters.

In the direction of quantum optics with molecules, we provide analytical models and solutions for the excitation migration between collective electronic levels in molecular aggregates and for processes involving non-radiative transitions due to non-adiabatic couplings of potential electronic landscapes in single large organic molecules.

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NOTES

INVITED TALK

Arrays of quantum dots or rings in a FIR-photon cavity

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We model both the dynamic and static effects of the interaction of a two-dimensional electron gas (2DEG), in a periodic array of quantum dots or rings, with the photons of a cylindrical TE011 (far-infrared) FIR cavity mode. The 2DEG in the array is in an external homogeneous magnetic field in a GaAs heterostructure.
The Coulomb interaction between the electrons is described by a spin-density functional approach, but the para- and diamagnetic electron-photon interactions are modelled *via* a configuration interaction formalism in a truncated many-body Fock-space, which is updated in each iteration step of the density functional approach. The time-dependent excitation of the system is accomplished by a coupling scheme to a cylindrical cavity mode for emphasizing the diamagnetic electron-photon interaction not leading to simple electrical dipole oscillations. The diamagnetic interaction is enhanced by the rotational electric field of the TE011 cavity mode. The interaction of the cavity field affects the polarization of the 2DEG. We observe two-photon diamagnetic transitions and higher order harmonics thereof. Generally, the electron-photon interactions reduce the Coulombic exchange forces and we discover a situation where the spin-configuration of the 2DEG can be controlled by the electron-photon interactions.

References:
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NOTES

INVITED TALK – online presentation

Exploring CuAgZr metallic glasses for biomedical use: A study using combinatorial synthesis, high-throughput experiments, and machine learning

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This study focuses on CuAgZr metallic glasses (MGs), which are notable for their potential in biomedical applications thanks to their exceptional strength, resistance to corrosion, and antibacterial properties. By employing a synergistic approach that combines combinatorial synthesis, high-throughput characterization, and machine learning, we have conducted a thorough examination of the mechanical attributes of CuAgZr MGs. Our findings indicate that the presence of high oxygen levels in Cu-rich areas, resulting from post-deposition oxidation in regions of less dense packing, markedly influences the mechanical performance of these alloys. Additionally, our research uncovers that nanoscale structural nuances play a significant role in determining the plastic yield and flow behavior of the alloys. Among various machine learning models evaluated, the multi-layer perceptron algorithm stood out, delivering accurate predictions of hardness for alloys not previously tested, thereby offering insightful directions for ongoing material research. This investigation underscores the efficacy of leveraging combinatorial synthesis, high-throughput analysis, and machine learning to accelerate the development of new metallic glasses with enhanced mechanical properties and cost-effectiveness.

NOTES

INVITED TALK

Hybrid perovskite materials: From perovskite solar cells to memristive elements

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The hybrid perovskite materials have been in the focus in the past few years for the rapid surge in power conversion efficiency obtained in perovskite solar cells (PSCs), which is presently at 26.7%. This is similar to the standard silicon technology, while the fabrication costs of PSCs are typically more reduced, taking advantage of the chemical synthesis routes. In spite of these developments, the stability of the perovskite materials requires further improvement. One important factor that induces PSC degradation is the ion migration, which is also identified in the peculiar capacitive and inductive phenomena observed in the electrochemical impedance spectroscopy measurements [1]. However, finding optimal perovskite materials is not an easy task. To this end, new approaches have been developed, which combine ab initio calculations with machine learning techniques, allowing an efficient exploration of the compositional space [2]. This outlines the role of the organic cations and of the halogen mixtures, which are confirmed experimentally [3]. More recently, it was realized the ion migration in hybrid perovskites can be exploited in the fabrication of memristive elements and this phenomenology can be suitably analyzed using equivalent circuit models. Hybrid perovskite memristors would therefore close the loop, as memristive elements can be employed in further material discovery.

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NOTES

Abstracts
of
Poster Presentations

POSTER PRESENTATION ***P1***

Predicting the structure of chalcogenide compounds using machine learning

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Chalcogenide glasses (ChGs) exhibit remarkable electrical and optical properties, enabling their applications in optical fibers, solid-state batteries, thermal imaging devices, and ovonic threshold switches [1]. With increasing integration of artificial intelligence in materials science [2], this study focuses on employing machine learning techniques to predict new, homogeneous, and stable ChGs. Consequently, we compiled an extensive dataset comprising approximately 58,000 chalcogenide compounds extracted from the SciGlass database [3]. We employed ten machine-learning models for a binary classification to distinguish between glassy and non-glassy materials. This selected models includes k-nearest neighbors, random forest, extreme gradient boosting, histogram-based gradient boosting, light gradient-boosting machine, extremely randomized trees classifier (ExtraTrees), adaptive boosting of decision trees, and categorical boosting. Additionally, two meta-models, Voting and Stacking Classifiers, were trained using predictions from these base models, achieving significant performance enhancements. Results highlight the potential of machine learning for glass-forming materials classification. After hyperparameter optimization, all models achieved high performance, with the F1-score exceeding 85%, Matthews correlation coefficient surpassing 65%, and Receiver Operating Characteristic - Area Under the Curve (ROC-AUC) scores greater than 83%. Several models also demonstrated robust extrapolation capabilities when applied to an independent experimental dataset consisting of 417 magnetron co-sputtered thin-film compositions, primarily outside the collected original bulkglass focused database. Notably, the ExtraTrees model excelled with an accuracy of 67% and ROC-AUC score of 70% for this validation set. Subsequently, SHAP (Shapley additive explanations) analysis was conducted on topperforming models to elucidate the influence of theoretical physical and chemical parameters on glass-forming ability in chalcogenide materials. This analysis highlighted distinct differences between chalcohalide glasses and simple chalcogenide glasses, particularly regarding valence electron configuration attributes.

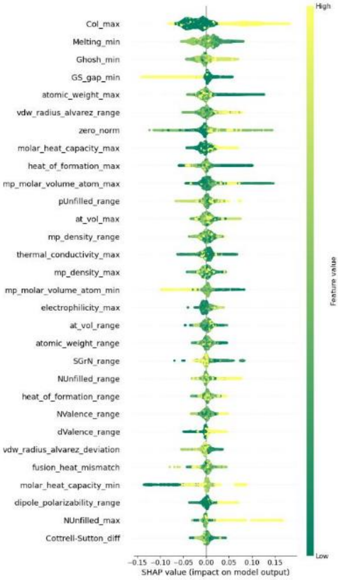

Fig. 1: SHAP feature importance ranking from the ExtraTrees model

References:

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POSTER PRESENTATION ***P2***

Customized graphene-like materials for sensing volatile organic compounds

Calin-Andrei PANTIS-SIMUT[1,2], Mihaela COSINSCHI[1,2,3,*], Alaa ALLOSH[1,2], Nicolae FILIPOIU[1,2,3], Amanda Teodora PREDA[1,2], Camelia VISAN[2], George NECULA[2], Ioan GHITIU[4], George Alexandru NEMNES[1,2,5]
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Phosphorene and MoS_2 are two graphene-like materials with tunable properties that have been employed in a wide range of applications. Sensing volatile organic compounds (VOCs) associated with different respiratory diseases is highly important for a rapid diagnosis.

To this end, phosphorene and MoS_2 active layers are customized with substitutional impurities from group-IV, group-VI and transition metal elements to create binding centers [1]. The binding capacity of several biomarkers specific to tuberculosis, nosocomial pneumonia, Aspergillus fumigatus, influenza and SARS-CoV-2 virus infections is assessed and confirmed by molecular dynamics simulations. Introducing a pattern based approach using multiple biosensing device elements, we prove a considerable selectivity for the five biomarker compounds. In addition, we take into account perturbing factors stemming from the background compounds like H_2O, CO_2, O_2, N_2 that would normally appear in the exhaled air.

We investigate several configurations of attached molecules in the framework of a multi-scale model. Finally, we investigate the electric field effect on the conductance modifications of the biosensing elements with molecules attached

Reference:

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POSTER PRESENTATION ***P3***

Capacitive and inductive effects in perovskite solar cells and memristor devices

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Iodine migration has been evidenced in hybrid perovskites and its connection with the hysteretic phenomena in perovskite solar cells is well established. In recent years, the origins of rather peculiar capacitive and inductive effects were highly debated. Currently there is a large consensus that ions are responsible for a dephased recombination. Using a special Ansatz for the recombination current, which is modulated by the ionic current and ionic charge, we show that the internal electric field and ionic-induced defects are responsible for the capacitive and inductive effects, respectively [1].

In photovoltaic technology, understanding ion migration is important for identifying and mitigation of possible degradation pathways. However, the detrimental effect of ion migration in perovskite solar cells can be turned into an advantage, playing a central role in the realization of memristor devices [2]. Using equivalent circuit models we show roles of capacitive and inductive effects in establishing the memristor I-V characteristics.

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POSTER PRESENTATION ***P4***

Finite Element design of a magnetic device for limiting sedimentation of nanoparticles in a viscous fluid

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The integration of magnetic nanoparticles (MNPs) into clinical practice has been explored in various contexts, including drug delivery, magnetic resonance imaging contrast enhancement and hyperthermia treatment for cancer. However, a general problem in any context is targeting the desired tissue by MNPs, together with a proper control against their sedimentation in a viscous-like fluid. It is magnetophoresis the branch of physics which deals with the motion of magnetic particles or bodies in a fluid under the influence of a magnetic field gradient. It is relevant not only in biomedicine (e.g., magnetic separation, target drug delivery) but also in colloidal science, and microfluidics. The key equations governing magnetophoresis, assuming a Newtonian fluid and low Reynolds number regime (Stokes flow) are related to the magnetic force (F_{mag}) and the Stokes drag force (F_{drag}) acting on the MNP, as effect of the field gradient and of the viscous resistance of the fluid, respectively:

$$\vec{F}_{mag} = \frac{V_p}{\mu_0}\chi_{eff}(\vec{B}\cdot\vec{\nabla})\vec{B} = \nabla(\vec{\mu}_p\cdot\vec{B})$$

$$\vec{F}_{DRAG} = 6\pi\eta r\vec{v}$$

where $\vec{B}$ is the magnetic induction of the applied field, V_p is the volume of the particle, χ_{eff} is the effective magnetic susceptibility, $\vec{\mu}_p$ is the magnetic moment of the particle, $\vec{v}$ is the particle velocity, r is the radius of the nanoparticle and η is the dynamic viscosity of the medium. When discussing about sedimentation under gravitational forces, also the apparent weight of the MNP should be considered. The full magnetophoretic problem, including inter-particle interactions, can be solved only numerically in either more simplified cases or by using finite element algorithms implemented in commercial programs as for example COMSOL Multiphysics which is able to provide also the magnetic configuration associated to geometrically distributed permanent magnets. The sectional distribution of the magnetic fields and of the magnetic forces for a configuration of 2 permanent magnets of NdFeB making an angle of 90 deg with symmetrical orientation versus the vertical direction and North and South poles facing each other, is presented in Fig.1. as exemplification. This configuration has been designed for a specific device devoted to reduce the sedimentation of magnetic nanoparticles keeping them without agglomeration for longer time (about 20 times longer than in the absence of the device) in a well localized volume.

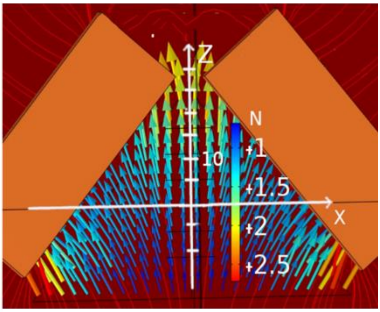

Fig. 1: Spatial distribution of magnetic forces as generated by a configuration of two permanent magnets represented in the figure by rectangles. The configuration is designed for reducing sedimentation velocity of MNPs in a viscous medium.

POSTER PRESENTATION ***P5***

A DFT study of phosphorene functionalized with RGO for drug detection sensors

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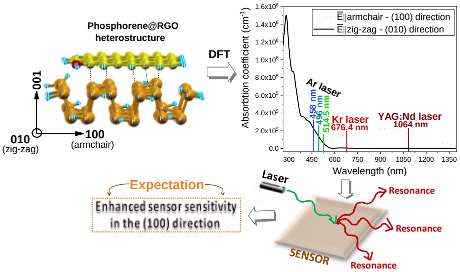
Phosphorene has garnered significant attention in the research community for its potential applications in sensing and optoelectronic devices [1]. This interest is attributed to the material's anisotropic properties and its capacity for efficient functionalization, which is facilitated by its structural characteristics [2,3].

In this study, DFT calculations were utilized to investigate the anisotropy of phosphorene and its heterostructures with RGO, as determined by their optical properties, in the context of optical sensors for drug detection. Two types of phosphorene@RGO heterostructures were analyzed: (i) covalently functionalized systems with P-C bond formation and (ii) non-covalently stabilized systems through van der Waals interactions. The optical responses of both pristine and functionalized phosphorene under polarized light were correlated with their electronic structures, including the density of electronic states and the distribution of molecular orbitals. The present investigation is founded on the anisotropy of phosphorene in the armchair and zig-zag directions, as previously demonstrated by an experimental study of polarized Raman scattering [2].

It is crucial to understand the optical anisotropy of phosphorene@RGO heterostructures for the development of high performance drug sensing sensors. These properties significantly influence the drug sensing mechanisms and the sensitivity of the sensor platforms depending on the direction of the applied optical vector. The present results provide insights into the electronic and optical changes induced by phosphorene functionalization, which is pivotal for the optimization of these platforms. At the same time, the comparative analysis between covalent and non-covalent functionalization strategies offers valuable guidance for the design of heterostructures for drug detection.



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POSTER PRESENTATION ***P6***

3D tight-binding model for second-order topological insulators and quantum anomalous Hall effect

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We propose a 3D tight-binding model that exhibits the spectral properties of a second-order topological insulator (SOTI) and the transport characteristics of the quantum anomalous Hall effect (QAHE). The model consists of stacked square diatomic layers with Chern insulator properties, governed by next-nearest-neighbor hopping t_2, intralayer phase γ, and interlayer coupling $\gamma_\perp$. We analyze bulk, slab, and wire geometries, demonstrating that next-nearest-neighbor hopping controls the transition between semimetallic and topological insulating phases. Additionally, we examine the impact of boundary conditions on a slab system with varying surface atom connectivities and provide an analytical demonstration of zero-energy surface states in specific configurations. In the wire geometry, a gap emerges in the surface state spectrum, hosting hinge states of opposite chirality, indicating that a 3D QAHE can be realized. By simulating a four-terminal Hall device, we show that the number of layers influences hinge-state pathways, leading to distinct quantized Hall resistance values. Our findings emphasize the crucial role of symmetry, boundary conditions, and topology in the emergence of higher-order topological phases.

POSTER PRESENTATION ***P7***

Predicting 2D and 3D charge densities for quantum many-body systems

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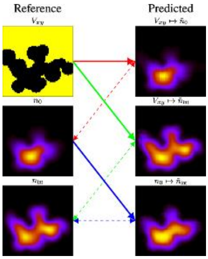
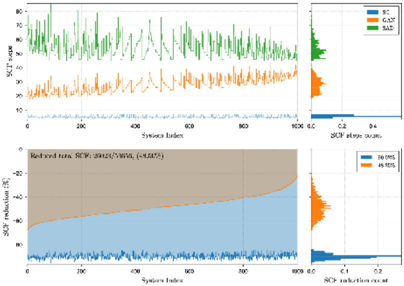
Quantum systems are shaping modern information processing technologies and designing them is one of the most outstanding challenges in modern physics. These systems are fairly complex due to the Coulomb interaction between the particles. There are several methods for solving such problems depending on the size (i.e. number of particles). For the interacting systems with several fermions, the most accurate solution is provided, beyond mean-field approaches, by the Exact Diagonalization (ED) procedure, which is regarded as the golden standard. For larger systems, other approaches, such as density functional theory (DFT), can provide an atomistic description by means of an effective oneparticle potential. The complexity that emerges in these systems can also be captured by machine learning techniques. In this work, we propose to bypass the numerical intensive computations from ED and DFT, by predicting the ground state charge densities using conditional Generative Adversarial Neural Networks (cGANs), which proved to be very efficient in image segmentation [1]. The first part consists of predicting the ground state of interacting and non-interacting charge densities of a fewelectron (i.e. N = 1,2,3,4) two-dimensional system in the presence of an external potential [2]. Taking advantage of the cGAN method, the inverse problem can also be solved. Several results are displayed in the left-hand side figure. In the second part, we use the same method to predict the self-consistent charge density from the super-position of atomic orbitals (SAD) that is initially used in the selfconsistent loop. The aim is to reduce the number of SCF iterations in the DFT procedure. The analyzed systems are composed of two classes, the first are isolated organic molecules, while the second ones correspond to silicon (Si) supercells with a number of vacancies. The results for the Si structure are depicted in the right-hand side figure, showing on average a 48.25% reduction in the number of SCF steps.





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*POSTER PRESENTATION **P8***

Floquet topological spin filters

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Floquet topological insulators are materials which undergo topological phase transitions caused by a time periodical driving which breaks the time reversal symmetry. In recent years, it was demonstrated that circularly polarized light irradiation triggers Floquet topological phases. Moreover, if an intrinsic spin-orbit coupling is present, due to light irradiation, an interesting interplay between spin and charge quantum Hall effect takes place. Here, we demonstrate that besides the two aforementioned topological phases, light irradiation may give rise to a spin filter phase, in which only one spin state is transmitted through the system. The main ingredient of our proposed mechanism of spin filtering is the presence of an on-site staggered potential which breaks the spatial inversion symmetry.

POSTER PRESENTATION ***P9***

Implementation of quantum sorters using trivial and topological materials within the BHZ model

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Along with the advent of quantum information within the last decades, the idea that we could harness quantum effects such as interference and entanglement in electronic devices has been the main objective in information technology. The idea of a quantum sorter emerged in this field, as a means to measure qubits for information processing. Though in theory one can propose a universal quantum sorter for any arbitrary observable [4,5], experimental implementations were only explored in the field of quantum optics [1,2,3]. In our work, we propose a solid-state version of a quantum sorter, based on a multi-terminal mesoscopic device with multiple output ports, that aims to separate the incoming states by both their spin and transversal mode. By choosing a suitable Hamiltonian in the scattering region, which can be controlled by electrostatic gates, we simulated a device that enables the separation of eigenstates into the four output leads. To this end, we used the R-matrix formalism [6] and Kwant [7], a tight binding based Python program, to model the proposed device. Also, in order to maximize the state-separation efficiency of the system, we chose to exploit the unique transport properties of topological insulators. We modeled a device that meets the criteria of an irreversible quantum sorter, employing the well-established BHZ Hamiltonian [8] to simulate a multi-terminal quantum system made up of both trivial and topological materials.

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POSTER PRESENTATION ***P10***

Micromagnetic simulations of nano-wires systems for permanent magnet applications

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We performed a systematic study of the influence of intrinsic material properties and of the size effects on the properties of magnetic nano-wires in AlNiCo magnets using micromagnetic simulations. Geometries are generated via the open- source computer- aided design (CAD) software Salome [https://www.salome-platform.org/]. The simulations use the finite element method to compute the magnetization distributions along the demagnetization curves. The micromagnetic solver applies a preconditioned conjugate gradient method for energy minimization [1]. We analyzed magnetic wires with different diameter, aspect ratio, tip end shape and wire interspacing. The intrinsic magnetic properties of the rods were taken from literature [2]. To validate the simulation results, we designed the wire geometry and orientation distribution of the long axes of the rods based on transmission electron microscopy images and on demagnetization curves measured via a closed-loop method. Using the ratio of remanent magnetization to saturation magnetization taken from experiments, we estimated the standard deviation of the orientation distribution of the long axes of the rods. The coercive field is determined by the rods oriented at the angle that corresponds to the maximum of the angular distribution [3]. Figure 1 shows a sketch of the wires setup considered and the comparison between simulated and measured coercivity.

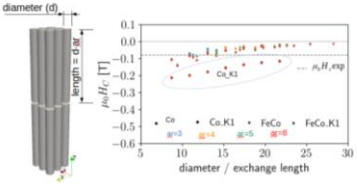

Figure 1. FeCo wires setup (a). The coercive field as a function of combined parameter rod diameter and exchange length for different materials and aspect ratios (ar). The dashed line gives the experimental coercive field (b).

Results from several hundred simulations were collected and used for training a machine learning model that gives the coercive field as function of the spontaneous magnetization, the rod diameter, the aspect ratio, and the misorientation angle of the rod with respect to the alignment direction.

We analyzed the dependence of the magnetic properties on rod dimensions based on the interplay between shape anisotropy and magnetostatic interactions. Magnetostatic interactions reduce loop squareness. The coercivity of these systems can be enhanced by magneto-crystalline anisotropy and by adjusting the shape and the packing fraction. Quasi-uniform switching specific to rounded ends increase coercivity. The longer and thinner the needles are, the higher is the coercive field. Increasing the aspect ratio beyond 8 does not enhance coercivity, but at a fixed aspect ratio, coercivity increases as the diameter decreases. The coercive field is around µ0Hc = 0.08 T for rod diameters of 22 nm. The corresponding energy product is 60 kJ/m^3.

Acknowledgments:
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POSTER PRESENTATION ***P11***

A band ferromagnetism model consistent with experimental observations – and some surprising predictions of it

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A consistent theory of ferromagnetism which accounts for most basic observed phenomena is still lacking. Amongst fundamental hypotheses, the localization of valence electrons responsible for the material's magnetic moment comes in a first place. Thus, two basic models were discussed to date:
(1) Models starting with electrons completely localized on atomic sites, where the overall atomic magnetic moments interact reciprocally. Leaving apart the dipole-dipole interaction, which should not favor ferromagnetic ordering, the most accepted hypothesis is that of inter-site exchange interaction by introducing the Heisenberg Hamiltonian $H_{12} = -2J_{12}\boldsymbol{S}_1 \cdot \boldsymbol{S}_2$. The origin of this interaction stems in the Heitler-London model of the hydrogen molecule, most precisely in the difference between the lowest-lying singlet and triplet electronic states. The introduction of the scalar product between the spins $\boldsymbol{S}_{1,2}$ is a forced extrapolation, as does the assumption that a similar behavior is to be expected for dimers of many-electron atoms and, further, to extrapolate this finding for a solid. (Not to speak that the Heitler-London model is itself an approximation.) Another unjustified information widely present in the community is the dependence of the exchange interaction J_{12} on the distance between the neighbors 1 and 2 for different metals, with positive values for ferromagnetic metals and negative for metals which do not show ferromagnetism with enough elevated Curie temperature: the "Bethe-Slater curve" which, at its origin, was only qualitatively argued [1]. The most popular model of ferromagnetism employs the mean field theory starting with the Heisenberg hamiltonian to derive the equation of state $M(B_a, T)$, where M is the magnetization, B_a the applied field and T the temperature. This model has the merit to predict Curie temperatures related to the strength of the exchange interaction $k_{\mathrm{B}}T_{\mathrm{C}} \sim J$, the occurrence of hysteresis in the ferromagnetic state, the variation of the susceptibility in the paramagnetic state $\chi \propto (T - T_{\mathrm{C}})^{-1}$, but for the coercive field at low temperature a too elevated value is predicted, since $\mu_{\mathrm{B}} B_a^{(c)} \sim J$. For $J \sim 0.1$ eV, this means $B_a^{(c)} \sim 10^3$ T. Other models relying (also) on localized electrons, such as the RKKY model [2] suffer on the same basic inconsistency. To circumvent this difficulty, the community mixed the above described Curie-Weiss theory based on the Heisenberg interaction with a phenomenological Stoner-Wohlfarth model involving magnetic anisotropy and rotation of the magnetization between the axis of the magnetic anisotropy and the direction of the applied magnetic field [3]; this model also predicts hysteresis, and the coercive field is proportional to the atomic anisotropy energy which is then supposed to have values on the order of □eV/atom to yield $B_a^{(c)} \lesssim 0.1$ T. Hence, when one speaks about temperature variations, Curie temperatures, or susceptibilities one invokes the Curie-Weiss model, and when discussing about coercive fields one uses the (completely different, and mostly qualitatively grounded) Stoner-Wohlfarth model. Also, microscopic determinations of magnetic anisotropy energies by X-ray magnetic dichroism yield values two orders of magnitude larger than those supposed above to match the observed values of the coercive fields, i. e. 0.2–0.4 meV/atom [4].
(2) Models starting with localized electrons, i. e. the band ferromagnetism. The 'standard' one is the Stoner model [4], where one supposed the density of states (DOS) of the metal split between two sub-bands ("majority" or spin ↑, and "minority" or spin ↓). A stabilization energy density proportional to the squared difference between the electron density in the majority and minority subbands $n_{\uparrow,\downarrow}$ is proposed and may be argued based on the Hubbard model, or on the empirical consideration of the Coulomb intra-site repulsion of electrons U with opposite spins, i. e. $\Delta w_s = -U(\Delta n)^2/n_0$, where $\Delta n = (n_\uparrow - n_\downarrow)/2$ and n_0 is the density of all available electronic states (twice the atomic density) [5]. The transfer of Δn electrons per volume unit from the minority towards the majority states comes with an excess of kinetic energy which can be written (in terms of energy density) as $\Delta w_k = (\Delta n)^2/\{g(\varepsilon_{\mathrm{F}})n_0\}$, where $g(\varepsilon_{\mathrm{F}})$ is the DOS at the Fermi level in the paramagnetic state. From the condition that the ferromagnetic state is lower in energy one obtains the well-

known Stoner criterion $g(\varepsilon_{\mathrm{F}})U > 1$. Although the model is a drastic approximation of metals with several valence electrons per atom (in fact, the Hubbard model supposes that on each site only two electrons with opposite spins may be accommodated) and also it yields unreasonably high Curie temperatures $k_{\mathrm{B}}T_{\mathrm{C}} \sim J \sim \mathrm{eV}$, the Stoner criterion is still widely used in assessing the ferromagnetism in metals.

Hence, the models discussed previously start on completely different theoretical grounds, each one of them comprises drastic approximations and all are used concomitantly in the world of magnetism!

In this Communication, I will discuss an improvement of the Stoner model based on the simple assumption that the *total* energy Δw_t should be compared between the ferromagnetic and the paramagnetic state of the metal and not only the kinetic energy (i. e. one should take into account the shift of the bottom of the conduction band towards lower energies for spins ↑ and towards higher energies for spins ↓, the Feri level being the same for both sub-bands). It follows that for a constant DOS any system should evolve towards the state with maximum spin asymmetry. For non-constant DOS, the computation of the susceptibility at zero magnetization $\chi(0) \propto [\partial^2 \Delta w_t / \partial(\Delta n)^2]_0^{-1}$ yields the cases where the ferromagnetic state is the most stable (negative $\chi(0)$). This suggests a criterion for ferromagnetism relying only on the DOS, which is on the form $(dg/d\varepsilon)(\varepsilon_{\mathrm{F}}) \int_0^{\varepsilon_{\mathrm{F}}} g(\varepsilon) d\varepsilon < g^2(\varepsilon_{\mathrm{F}})$ [6]. In a simplified view, metals with descending DOS as function on the energy $(dg/d\varepsilon)(\varepsilon_{\mathrm{F}}) < 0$ feature ferromagnetism. This model explains the ferromagnetism of 3d metals and also their most probable crystal structures, when combined with simple considerations from crystal field theory. Also, the temperature dependence can be easily introduced and, by using a simplified DOS, for Fe and Co reasonable Curie temperatures are predicted, in agreement with experiments. The model can also be easily extended to predict reasonably low coercive fields and their temperature dependence. And the most surprising findings occurs when one estimates the behavior at elevated temperatures, where, at least for bcc Fe and hcp Co, a “re-entrant” ferromagnetism is predicted (i. e., starting with a temperature, $\chi(0)$ becomes again negative). The temperatures where such phenomenon might be expected are of several thousand Kelvin (over 6,000 K for Fe) and no metal is expected to survive at those temperatures. However, the model could be applied to infer the ferromagnetic nature of the Earth’s inner solid core, which is mostly composed by hcp Fe at temperatures such as the ones discussed above. A detailed DFT computation at high pressures for hcp Fe, together with the application of the rigid shift model and with the introduction of the Fermi-Dirac distribution function yielded a similar result. The Earth’s inner solid core could be ferromagnetic at temperatures between 6,000 and 6,500 K and pressures of 2.5–3.5 GPa [7]. This suggest that the inversion of the magnetic poles can happen by simple rotation of the inner Earth’s magnet. As a consequence, the Earth’s surface will continue to be screened from solar radiation and no major extinction nor genetic mutations will happen. Note also that during the last about 200 million years several hundreds of geomagnetic field reversals occurred, with no drastic influence on the terrestrial lifeforms [8].

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POSTER PRESENTATION ***P12***

One- and two-dimensional models for ferromagnetic domains

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The aim of this Contribution is to revise Kittel's scaling law $l \propto d^{1/2}$ [1,2] where l is the domain width and d the film thickness, which is the cornerstone of micromagnetism [3]. This scaling law was obtained by using the approximation of a thick film with 180° stripe-like domains whose magnetizations are perpendicular to the film. In a first work [4], this one-dimensional theory was revised by going beyond the approximation used originally by Kittel, with two noticeable results: (i) For ultrathin films there are deviations from Kittel's scaling law, and for ultrathin films the domain width increases by lowering the film thickness. The turning point is defined by a 'critical thickness' $d_0 = \pi^3 w_{\text{wall}}/\left(4\mu_0 {M_0}^2\right)$, where w_{wall} is the energy associated to domain walls per unit area (of the wall), μ_0 the vacuum permeability and M_0 the magnetization inside each wall. For usual samples, d_0 is in the range of tens of nanometers. There is no need for suppositions such as the fractal dimensions involved in the domain structure [5]. (ii) A model was proposed with domains of different thicknesses when an external magnetic field is applied, to help computing the magnetization curves. The domain whose magnetization is parallel to that of the applied field has a larger thickness than the domain whose magnetization is oriented in the opposite direction. This model yielded no hysteretic behavior for infinite thin films (of finite thickness) and only by introducing demagnetization factors lower than unity, associated with the finite lateral size of the sample, may some hysteresis be predicted.

This work was refined further, by considering the two-dimensional case, i. e. domain structures as function of x and y, when the magnetization is oriented along the z direction. This allows the treatment of thin films with perpendicular magnetic anisotropy and also films with in-plane anisotropy [5]. The results were as follows: (i) For two-dimensional films with perpendicular magnetic anisotropy, the most stable structure for $\langle M \rangle = 0$ is found to be that with domains infinitely elongated along one in-plane direction, i. e. the one-dimensional case treated in the preceding work. (ii) For thin stripes with in-plane magnetization, the domain size l is approximately linear with the stripe *lateral* size d for low film thickness, while for large film thicknesses it follows a Kittel-like law, but as function of the stripe *lateral* size $l \sim d^{1/2}$. (iii) For in-plane magnetized thin films of infinite lateral extent, the most stable structure is the single domain. (iv) As for hysteresis curves, the two-dimensional case with perpendicular magnetic anisotropy is shown to evolve from a 2D landscape derived from the checkerboard structure, but with unbalanced domains for magnetization near saturation, towards one-dimensional domain structures for lower magnetization. (v) In some cases and depending also on the demagnetization factor, the one-dimensional case is not reached, and the film exhibit 2D structures on the whole range of the magnetization curve. (vi) The hysteresis obtained for thin magnetic stripes with in-plane magnetization also can exhibit a rich structure, with minor cycles on the wings of the magnetization curves evolving towards „normal" hysteresis (again, depending on the film thickness, stripe lateral size and demagnetization factor). (vii) An infinite thin film with in-plane anisotropy features a steplike magnetization dependence on the applied field.

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POSTER PRESENTATION ***P13***

Microscopic model of ferroelectricity and derivation of the equation of state within a standard mean field approach

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The standard approach in statistical mechanics is to start with a microscopic model for the most elementary constituents of the system investigated (atoms, molecules, individual moments, etc.) and then to elaborate the statistics of it, by using appropriate thermodynamic potentials and partition functions. Unlike the Curie-Weiss mean field theory of ferromagnetism which is based on the microscopic Heisenberg interaction between elemental atomic spins, until quite recently ferroelectricity lacked such a microscopic model. The "modern theory of polarization" proposed for ferroelectric phenomena by King-Smith, Vanderbilt and Resta in the early 1990s [1–6] went somehow in the opposite wish of a simple microscopic for ferroelectricity. It was stated that 'elemental' dipole moments are ill defined, except for extremely ionic materials [4,5]. The polarization itself of a piece of material is not uniquely defined, more specifically it is not a vector, but an array of vectors spaced by "polarization quanta". If the polarization is not well defined, only polarization differences ΔP represent, in fact, measurable quantities and may be related to time integration of the electric current flowing through the sample when the voltage applied to it is reversed adiabatically. Experimentally, this is the standard way to determine the ferroelectric polarization, e. g. through Sawyer-Tower circuits. Since electronic currents in a sample are related to phases of electronic wavefunctions, ΔPs may also be related to phases acquired when the system switches between two states, and this was related to early Berry's work on "quantal phase factors accompanying adiabatic changes" [7]. A sophisticated theory, involving "Berry connections", generalized Stokes theorem in a mixed space formed by the reciprocal space and the parameter of adiabatic changes, with relations to Born effective charges and displacement of Wannier centers was developed to help computational physics to predict polarization in ferroelectric crystals. Putting everything together, if the polarization of a crystal is not uniquely defined and, in any case, cannot be written as some kind of "elemental" dipole moment times the density of dipoles, there is no hope to develop a microscopic model for this phenomenon, nor its thermodynamics [8].

In 1993, Vanderbilt and King-Smith already stated a direct correlation between the polarization and the surface charge accumulated at external surfaces and interfaces of the material [2]. This accumulated charge was evidenced also by theoretical [9] and experimental [10] works as a consequence of the ferroelectric polarization, as follows: (i) for a single domain ferroelectric film with polarization oriented out-of-plane, the fixed charges at the extremities of the film generate a ‚depolarization field' strong enough to destroy the ferroelectric state; (ii) for thick films, the polar state of the material survives by the formation of 180° ferroelectric domains; (iii) however, experimentally, ultrathin ferroelectric films feature a single domain state; (iv) as a consequence, in the latter systems, an additional charge formed by mobile charge carriers from the volume of the material of opposite sign with respect to the ‚fixed' charges is needed near the external surfaces to compensate the depolarization field. It was taken into account that usual ferroelectric materials are quite often wide bandgap semiconductors instead of insulators. More refinements were proposed later, in the sense that the ‚compensating' charge can also be located in external electrodes or contaminants; also, even for free ultraclean ferroelectric surfaces these charge layers can also be formed by layers of ionized impurities from the semiconductor [11].

Recently, it was supposed that the ferroelectric material is still composed by some ‚elemental' dipoles (*e.g.*, dipole moments of distorted unit cells), and the interaction of such an elemental dipole with the rest of the polarized material vanishes for a large bulk sample [12]. What subsists is the interaction with charges accumulated at surfaces or interfaces of the material [2], and this interaction is on the form $-GpP/(\epsilon_0\kappa) = -Gpn_0\langle p\rangle/(\epsilon_0\kappa)$, where G is a dimensionless ‚geometric factor' depending on the film thickness (quite close to 0.5), p the value of the elemental dipole, $\langle p\rangle$ its average value, $P = n_0\langle p\rangle$ the polarization, n_0 the volume density of elemental dipoles, ϵ_0 the vacuum permittivity and κ the dielectric constant of the material. This energy is on the ideal form to be treated by mean field statistical mechanics in a formalism

similar to the Curie-Weiss theory of ferromagnetism. Equations of state are derived, with reasonable values for Curie temperatures and coercive fields, which is not the case for the standard theory of ferromagnetism [13,14]. A semantic dichotomy with respect to the previous model about the necessity of charges accumulated at surfaces and interfaces to *compensate* the depolarization field is then suggested: as soon as the material itself or the heterostructure where it is integrated may generate some charges at interfaces, this phenomenon happens and the respective charges are stabilizing the ferroelectric state. Charges accumulated at surfaces or interfaces are therefore not a *consequence* of the ferroelectric state, but its *origin*. Instead of *compensating* the depolarization field, these charges may be seen as *stabilizing* the ferroelectricity. This does not happen in any wide gap polar semiconductor simply owing to the value of the dielectric constant: if it is too low, the electric field needed to pole the material exceeds the breakdown field.
The parameters of this model are the maximum value of the elemental dipole p_0, their density n_0 and the dielectric constant κ, and they can be determined from experimental quantities such as the saturation polarization $P_0 = n_0 p_0$, the Curie temperature and the coercive field at zero temperature. A further refinement of this model was developed by supposing the non-constancy of the material permittivity. In fact, one can define ‚static' of ‚dynamic' permittivity, which may be derived from the equation of state by computing the susceptibility and taking into account the poling history of the sample [13]. It turned out that for a consistent agreement with experimental data one still needs to use another input parameter, which is the ‚background dielectric constant', which may then be derived from experimental data (saturation polarization, coercive field, Curie temperature). The good prediction of this model with variable permittivity was the linear decrease of the coercive field with temperature, which is confirmed experimentally.

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*POSTER PRESENTATION **P14***

Unraveling symmetry breaking in perovskite oxides: A first-principles study of structural, thermodynamic, and electronic properties

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The family of ABO_3 perovskite oxides have been explored extensively over the century for their potential technological and energy applications. Thanks to their robust structural framework, which enables stabilization of diverse compositions and can lead to interesting properties [1]. Following Goldshmidt tolerance factor, the ABO_3 system can adapt cubic, hexagonal, tetragonal or orthorhombic phase [2]. These symmetric phases form predominant structural models for most of the scientific works done till date. However, scientific works exploring disorders in perovskites such as octahedral tilting, broken symmetry in BO6 octahedra, *etc.* is relatively scarce [3–6]. And their impact on different physical properties across different compositions remain yet to be understood.

In this work we aim to understand the implications of different disorders on structural, thermodynamic and electronic properties via first-principles simulations (DFT). We generate representative disordered structural models by adapting symmetric structural templates, disordered structural templates [6] and introducing random perturbations. *Via* systematic *ab initio* exploration of such models on representative composition $CaZrO_3$ and $BaTiO_3$, we obtain significant increase in thermodynamic stability and alteration of band gaps of disordered structures as compared to cubic phase. Based on these findings, we further explore the larger family of perovskite oxides to elaborate on the influence of disorder on different physical properties.

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POSTER PRESENTATION ***P15***

ApeironAI: The AI-powered workflow orchestrator for efficient material simulation

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ApeironAI is an innovative platform aimed at streamlining and accelerating workflows for the design and engineering of advanced materials. The platform integrates seamlessly with *ab initio* computational tools, such as Quantum ESPRESSO and SIESTA, in combination with AI agents, to automate and enhance the evaluation of physical properties in new materials.
As a first case studies we used amorphous boron nitride and graphene structures.
ApeironAI also leverages a linear-scaling methodology [1] to handle computations of large atomic systems, allowing simulations of large systems.
Core Technologies and Methods:

- AI Models:
  - Graph neural network (GNN) architectures ensure scalability and effectively manage complex molecular relationships.
  - Large language models (LLMs) are utilized for hyperparameter optimization and training tools.
- Computational Tools: Integration with Quantum ESPRESSO and SIESTA enables robust and accurate *ab-initio* computations.

ApeironAI enable faster and smarter workflows, helping both researchers and industries advance material simulation.

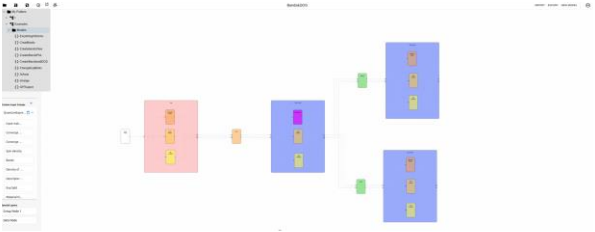

Fig. 1*: Workflow for computing Bands and DOS.*

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