CMT*a***BRIXEN**

28th-30th August 2024

The Meeting of the Condensed Matter Theory Italian Community

PROGRAM & BOOK OF ABSTRACTS



Università degli Studi di Padova





ALMA MATER STUDIORUM Università di Bologna



UNIVERSITÀ DI PARMA



ADVANCING SOLID INTERFACES AND LUBRICANTS BY FIRST PRINCIPLES MATERIALS DESIGN













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Program

Tuesday the 27th of August 2024

Welcome Dinner (20:00 – Hotel Grüner Baum)

Wednesday the 28th of August 2024

From 8.00 onwards Registration

Introductory Remarks (8:45 to 9:00)

Electronic Excitations and ultrafast Spectroscopy (9:00-12:50)

9:00-9:50 Keynote: Maurizia Palummo – Excited state properties of novel 2D/layered materials by ab initio DFT and MBPT methods

9:50-10:20 Invited: Francesco Macheda – First principles calculations of dynamical quadrupoles and higher order terms from the density response in large semiconducting and metallic systems

10:20-10:50 Invited: Pierluigi Cudazzo - Dynamical effects in the spectra of neutral excitations

Coffee Break (10:50-11:20)

11:20-11:50 Invited: Virginia Carnevali – Multi-scale simulations of photovoltaic devices based on organic halide perovskites

11:50-12:05 Contributed: Giovanni Caldarelli – How to screen electronic vertices of time-dependent response functions in hybrid functionals and Bethe-Salpeter equation approaches

12:05-12:20 Contributed: Manuel López Díaz – Fine-tuning electronic excitations in photoswitch quantum dot nanohybrid systems

12:20-12:50 Invited: Gianni Profeta - Doping a 2D Mott insulator: path to superconductivity

Lunchtime (12:50-14:30)

Magnetism, Ferroelectricity, Multiferroicity and Topology (14:30-18:20)

14:30-15:20 Keynote: Nicola Spaldin – Hunting for hidden order

15:20-15:35 Contributed: Matteo Cococcioni – Magnetic properties of octanuclear magnets from firstprinciples

15:35-16:05 Invited: Antimo Marrazzo – Taming spin-orbit coupling from first principles: electronic screening, topology, disorder and temperature

Coffee Break

16:35-17:05 Invited: Alessandro Chiesa – Modeling chirality-induced spin selectivity in electron transfer for quantum applications

17:05-17:20 Contributed: Federico Orlando – AMaRaNTA: an AiiDA-based workflow to automate calculations of exchange parameters in 2D magnets

17:20-17:50 Invited: Jagoda Sławinska - Spin-orbitronics in chiral crystals

17:50-18:20 Invited: Andrea Droghetti – First-principles electronic structure and quantum transport methods applied to spintronics

Poster Session 1 (18:20-19:30)

Dinner (20:00 – Ristorante Grissino)

Thursday the 29th of August 2024

Surfaces, Interfaces and 2D Materials (9:00-12:50)

9:00-9:50 Keynote: Carlo Antonio Pignedoli – Simulation challenges in the fabrication and characterization of quasi 1d carbon based nanostructures

9:50-10:20 Invited: Margherita Marsili – Developing tools in computational tribology for the highthroughput modeling of solid-solid interfaces

10:20-10:50 Invited: Davide Tisi – Transport properties of solid-state electrolytes at hybrid dft-level with machine learning

Coffee Break (10:50-11:20)

11:20-11:50 Invited: Silvia Bonfanti – Machine learning discovery in high entropy materials: derivatives of cantor alloys and complex glasses

11:50-12:05 Contributed: Andrea Corradini – A machine learning approach to light-induced orderdisorder phase transitions

12:05-12:20 Contributed: Ivan Rivalta – Modeling of gold nanobipyramids: from anisotropic growth to chiral properties

12:20-12:50 Invited: Massimo delle Piane – Exploring atomic dynamics in metals with molecular dynamics and machine learning

Lunchtime (12:50-14:30)

Quantum Science and Technologies (14:10-18:15)

14:10-15:00 Keynote: Simone Montangero – Tensor network algorithms for high-dimensional quantum many-body systems

15:00-15:15 Contributed: Chiara Capecci – Pulse-variational quantum eigensolver

15:15-15:45 Invited: Elisa Ercolessi - Hybrid variational algorithms on a neutral atom platform

15:45-16:15 Invited: Marco Govoni - Simulating spin defects in solids for quantum technologies

Coffee Break (16:15-16:45)

16:45-17:15 Invited: Leonardo Fallani – Strongly interacting lattice fermions: flavour-dependent mott localization and universal hall response

17:15-17:45 Invited: Matteo Michele Wauters – Analog quantum simulations of manybody systems with tunable josephson junction arrays

17:45-18:15 Invited: Luca Barbiero – Exploring strongly interacting fermionic quantum matter with magnetic atoms

Poster Session 2 (18:20-19:30)

Dinner (20:00 – Hotel Grüner Baum)

Friday the 30th of August 2024

Statistical Mechanics and emergent phenomena (9:00-12:50)

9:00-9:50 Keynote: Amos Maritan – Optimality and scaling in plants and forests 9:50-10:20 Invited: Ivan Di Terlizzi – Variance sum rule(s) for entropy production 10:20-10:50 Invited: Giuseppe Negro - Controlling flow patterns and topology in active emulsions

Coffee Break (10:35-11:05)

11:20-11:35 Contributed: Paolo Restuccia – Simulating reactions at sliding interfaces by ab initio and machine learning molecular dynamics

11:35-12:05 Invited: Vittoria Sposini – Being heterogenous is advantageous: extreme brownian nongaussian searches

12:05-12:35 Invited: Maria Chiara Angelini – A new renormalization group approach to disordered systems

Concluding Remarks (12:35-12:50)

ABSTRACTS OF TALKS

Wednesday the 28th of August 2024

Electronic Excitations and ultrafast Spectroscopy (9:00-12:50)

9:00-9:50 Maurizia Palummo (Keynote)

EXCITED STATE PROPERTIES OF NOVEL 2D/LAYERED MATERIALS BY AB-INITIO DFT + MBPT METHODS

Maurizia Palummo

INFN, Department of Physics, University of Rome "Tor Vergata"

The use of emerging two-dimensional and layered materials in technological applications presupposes a detailed knowledge of their chemical and physical properties. In this context ab-initio theoretical methods and simulations are playing a fundamental role.

Here I aim to show how the use of parameter-free atomistic simulations can contribute to improve the microscopic understanding of the opto-electronic properties of novel 2D materials and to predict new ones. I will show how ab-initio DFT and post-DFT (GW and BSE) calculations, based on Many-Body Perturbation Theory (MBPT), provide a very useful scheme to study i) the giant electronic band-gaps renormalization ii) the strong light-matter interaction iii) the presence of strongly bound excitons, iv) the exciton radiative lifetimes v) the influence of electron-phonon interaction on the electronic and optical spectra, vi) how doping and/or molecular functionalization can tune their opto-electronic properties. Among the families of 2D materials discovered after graphene, I will focus on those of particular interest for opto-electronic applications such Transition Metal Dichalcogenides (TMDs) as well as 2D/layered halide perovskites. Excitons of a recently proposed MoSi2X4 family will be also discussed.

Figure 1: square modulus excitonic wave function of a 2D material



M Palummo, S Postorino, C Borghesi, G Giorgi Applied Physics Letters 119 (5), 051103 (2021 C Quarti, G Giorgi, C Katan, J Even, M Palummo Advanced Optical Materials 12 (8), 2202801 (2024) LL Li, R Gillen, M Palummo, MV Milošević, FM Peeters Applied Physics Letters 123 (3) (2023) 9:50-10:20 Francesco Macheda (Invited)

FIRST PRINCIPLES CALCULATIONS OF DYNAMICAL QUADRUPOLES AND HIGHER ORDER TERMS FROM THE DENSITY RESPONSE IN LARGE SEMICONDUCTING AND METALLIC SYSTEMS

Francesco Macheda

Dipartimento di Fisica, Università di Roma La Sapienza, Roma, Italy

Within the context of first principles techniques, we present a theoretical and computational framework to determine the all-order quasimomentum expansion of the density response to an atomic displacement---Born effective charges, dynamical quadrupoles and octupoles etc.---in semiconductors and metals with large unit cells. Theoretically, we demonstrate that the density response in short-circuit conditions can be related to the screened one via a well-defined longrange dielectric function, even beyond the random phase approximation and in presence of nonlocal pseudopotentials. Our theoretical framework allows for a clever use of perturbation theory in the computational implementation, achieving a speed up of a factor of 3*Natoms with respect to the use of the 2n+1 theorem. We apply our developments to the computation of the piezoelectric properties of a large cell solid-solution of semiconducting hafniun oxide containing 96 atoms. We here show that the clamped ion piezoelectric response, which is determined solely by dynamical quadrupoles, can be decomposed into real-space localized contributions that mostly depend on the chemical environment, paving the way for the use of machine-learning techniques in the material search for optimized piezoelectrics. We further apply our methodology to determine the density response of metals. We here find that the leading terms of the charge expansion are related to the Fermi energy shift of the potential, if admitted by symmetry, and by Born effective charges which do not sum to zero over the atoms. These terms are then linked to the leading order expansion of the macroscopic electron-phonon coupling in metals. We apply our developments to the TEM-EELS spectroscopy of lithium intercalated graphites, where we find that approximating the density response via the use of the atomic form-factor in the long-wavelength limit does not take into account for the anisotropy of the atomic chemical bonding in the crystal.

ACKNOWLEDGMENTS

We acknowledge the MORE-TEM ERC-SYN project, grant agreement no. 95121.

DYNAMICAL EFFECTS IN THE SPECTRA OF NEUTRAL EXCITATIONS

Department of Physics, University of Trento, 38123 Povo, Italy

One of the big challenges of theoretical condensed matter physics is the description, understanding, and prediction of the correlation effects induced by the mutual interaction between particles on materials properties. In both electronic and optical spectra the Coulomb interaction and the electron-phonon coupling cause a renormalization of the energies and change of spectral weight. Most importantly, they induce a finite lifetime on the quasi-particle (QP) excitations and can lead to new structures, often called satellites. The latter are pure many body effects and can be linked to the coupling of excitations, also termed dynamical effects. Standard methods developed in the framework of many body perturbation theory namely GW and the Bethe-Salpeter equation (BSE)[1] are often not able to capture this complex physics. Instead, approaches based on a picture of electron-boson coupling such as the cumulant expansion are promising for the description of plasmon and phonon satellites.

Motivated by the recent success of the cumulant expansion of the one particle Green's function in the description of photoemission spectra[2,3,4], we generalized the cumulant approach to the evaluation of the electronic polarizability[5,6,7]. In this way we provide a new full ab-initio tool to include dynamical effects beyond the standard BSE in the description of neutral excitations as measured in optical absorption, photoluminescence, electron energy loss and inelastic X-rays scattering spectroscopies. The developed approach is applied to the study of phonon sidebands in the absorption and photoluminescence spectra of monolayer BN[8].

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11:20-11:50 Virginia Carnevali (Invited)

MULTI-SCALE SIMULATIONS OF PHOTOVOLTAIC DEVICES BASED ON ORGANIC HALIDE PEROVSKITES

Virginia Carnevali

Laboratory of Computational Chemistry and Biochemistry, Institute of Chemical Sciences and Engineering, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland

Hybrid inorganic halide perovskites (PSCs) have emerged as a promising class of materials for solar cells. Due to their remarkable optical properties, PSCs promote high power conversion efficiencies. Most of this rapid progress is due to changes in preparation conditions, while the fundamental understanding of the underlying processes at the atomic level is not necessarily present. In principle, computer simulation can elucidate the atomistic mechanisms underlying these phenomena, but the systems involved are very complex, with multiple atomic species and high activation barriers. My approach involves the development and application of multi-scale computational theoretical modelling spanning electronic and atomistic length scales. Classical molecular dynamics is complemented by ab-initio molecular dynamics and density functional theory at 0 K to obtain an accurate description of the physics behind the mechanisms responsible for the long-term stability and improved optical properties of PSCs, while also indicating possible new solutions for improved PSC devices.

ACKNOWLEDGMENTS

Swiss National Computing Centre CSCS (projects s1151 and s1253).

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11:50-12:05 Giovanni Caldarelli (Contributed)

HOW TO SCREEN ELECTRONIC VERTICES OF TIME-DEPENDENT RESPONSE FUNCTIONS IN HYBRID FUNCTIONALS AND BETHE-SALPETER EQUATION APPROACHES

Giovanni Caldarelli

Dipartimento di Fisica, Universita' di Roma La Sapienza, Roma, Italy

Incorporating excitonic and exchange effects into electronic calculations is crucial for accurately predicting the response properties of materials appealing to a wide range of applications. While hybrid functionals in DFT can partially capture exchange effects [1], excitonic effects in the response necessitate the use of Bethe-Salpeter equation (BSE) approaches [2,3]. Additionally, accurately accounting for the screening of the response function in interacting electronic systems remains a complex challenge, which has been explored in recent studies based on the time-dependent DFT (TD-DFT) [4,5].

In this work, we extend the TD-DFT linear response equations to include exact exchange, resorting to a density matrix formalism. This general approach encompasses different levels of linear response theory, such as TD-DFT with hybrid functionals, TD-Hartree Fock, and BSE within the statically screened exchange approximation. Our results provide a comprehensive methodology to compute electron-light and electron-phonon vertices within fully interacting response functions.

We demonstrate the effectiveness of our formalism by calculating the optical conductivity of graphene using a tight-binding model. Our findings show good agreement with experimental data and ab initio calculations, highlighting the accuracy and applicability of our approach.

ACKNOWLEDGMENTS

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12:05-12:20 Daniel López Díaz (Contributed)

FINE-TUNING ELECTRONIC EXCITATIONS IN PHOTOSWITCH-QUANTUM DOT NANOHYBRID SYSTEMS

Daniel López Díaz¹, Gabriel Gil², Stefano Corni², Guido Goldoni¹

Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università degli Studi di Modena e Reggio Emilia, Modena, Italia. Dipartimento di Scienze Chimiche, Università degli Studi di Padova, Padova, Italia.

Nanohybrid (NH) systems, combining semiconductor nanoparticles (NP) with organic photoswitch molecules (M), exhibit significant enhancements in electronic and optical properties compared to their individual components. This synergy is pivotal for applications in lighting, display technology, solar energy harvesting, and photodynamic therapy [1]. Our study focuses on refining and amplifying the excitonic properties of azobenzene (AB) when functionalized with a NP.

Simulating the electronic excitations in NHs, which typically encompass over 106 atoms, poses challenges with traditional first-principles methods. Conventional approaches often neglect electron correlation within and between fragments and suffer high computational costs when adjusting the NP size.

We employ the Hybrid Configuration Interaction (HyCI) method, an innovative approach able to accurately compute excitation energies and optical properties for NHs [2]. This method integrates first-principles simulations for the M, such as Configuration Interaction (CI) or Time-Dependent Density Functional Theory (TD-DFT), with CI under Effective Mass and Envelope Function Approximations (EM-EFA) for the NP. The spherical symmetry and angular momentum selection rules of the NP allows feasible computations at different sizes.

Applying the HyCI method to the AB+NP system, we analyze and compare energies, oscillator strengths, and absorption spectra of the NH with those of AB alone across varying reaction coordinate values during the trans-cis isomerization process. Our findings illustrate the capability to fine-tune electronic excitations in the photoswitch molecule through NP functionalization, highlighting the HyCI method's versatility and adaptability across diverse NP sizes and materials.

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DOPING A 2D MOTT INSULATOR: PATH TO SUPERCONDUCTIVITY

Gianni Profeta

Department of Physical and Chemical Science, University of L'Aquila (Italy)

Phenomena typical of two-dimensional correlated electron systems, such as unconventional superconductivity, metal-insulator transitions, commensurate charge density waves and unusual magnetic ordering have been observed triangular adatom lattices on semiconductor surfaces, like Sn/Si(111), Sn/Ge(111) and Pb/Si(111). From the structural and electronic point of view these two-dimensional systems are much simpler than other 3D systems materials which show the same behaviors, such as the cuprates, and therefore they are favorable models to test our understanding of the rich physics that arises from the interplay between Mott-Hubbard states, superconductivity, charge ordering, magnetism, geometric frustration, and doping.

Sn/Si(111)-(\sqrt{3}X\sqrt{3})R30 is confirmed to have a Mott-Hubbard insulating ground-state if undoped and undergoes a metal-insulator transition with temperature. Recently, hole-doping obtained by B acceptors, was found to drive the system back in the metallic phase joined by a pseudogap phase, which eventually become superconductor below about 4 K.

In talk, I present a complete experimental and theoretical investigation of the electronic properties of the B-doped phase of Sn/Si using ARPES supported by local probes of the surface like STS/STM, first-principles calculations of the realistic doped phases and model calculation including electronic correlations and inhomogeneities of doping, finding unexpected phenomena which question the common beliefs on the physics of surface doping.

Magnetism, Ferroelectricity, Multiferroicity and Topology (14:30-18:20)

14:30-15:20 Nicola Spaldin (Keynote)

HUNTING FOR HIDDEN ORDER

Nicola Spaldin

Department of Materials, ETH Zurich

Most magnetic materials, phenomena and devices are well described in terms of their constituent magnetic dipoles. There is mounting evidence, however, that higher-order magnetic multipoles can lead to intriguing magnetic behaviors, which are often attributed to "hidden order" since they are difficult to characterize with conventional probes. In this talk I will focus on the existence and relevance of the so-called magnetoelectric multipoles, which form the next-order term, after the magnetic dipole, in the multipolar expansion of the energy of a magnetization density in a magnetic field. I will describe how magnetoelectric multipoles underlie multiferroic behavior and dominate the magnetic response to applied electric fields, then discuss signatures of hidden magnetoelectric multipolar order and possibilities for its direct measurement. I will argue that all is not lost if your material lacks magnetoelectric multipoles, and that hidden magnetic octupoles and even triakontadipoles also cause fascinating physics, including the currently rather fashionable "altermagnetism". Finally, I will show that ferroic ordering of these higher-order magnetic multipoles results in a magnetization at the surface of a sample, even in materials with no net magnetization in their bulk and with apparently compensated surface dipoles.

15:20-15:35 Matteo Cococcioni (Contributed)

MAGNETIC PROPERTIES OF OCTANUCLEAR MAGNETS FROM FIRST-PRINCIPLES

Matteo Cococcioni

Department of Physics, University of Pavia

Molecular nano-magnets are systems of great technological appeal for applications that range from spintronics to quantum information. This work presents a computational study of the magnetic properties of some ring-shaped molecular nano-magnets, each containing eight transition-metal atoms, such as Cr8, and V8. Ab initio calculations, based on Hubbard-corrected non-collinear spin DFT, are used to calculate the effective exchange interactions (including effective Dzyaloshinskii-Moriya couplings) between the magnetic centres, through the sampling of selected spin configurations and a thorough comparison of their energies. The couplings so obtained are then used to construct a generalised Heisenberg Hamiltonian whose diagonalization gives direct access to the ground state of these systems, their low-energy spectrum, their finite-temperature susceptibility and other interesting properties. While the antiferromagnetic ground state of Cr8 is confirmed, the V8 shows an unusual ferromagnetic ground state characterised by a remarkable anisotropy and a high susceptibility to doping as demonstrated by our preliminary results on V7Ni. Results from the ring-shaped molecules are also contrasted with those from their linearised counterparts of equal composition, to highlight the role of the curved geometry.

15:35-16:05 Antimo Marrazzo (Invited)

TAMING SPIN-ORBIT COUPLING FROM FIRST PRINCIPLES: ELECTRONIC SCREENING, TOPOLOGY, DISORDER AND TEMPERATURE

Antimo Marrazzo

Scuola Internazionale Superiore di Studi Avanzati (SISSA), via Bonomea 265, 34136 Trieste, Italy

The presence of spin-orbit coupling or non-collinear magnetic spin states can have dramatic effects on the ground-state, topological and spectral properties of materials. While non-collinear densityfunctional theory calculations have become routine, the computational design, discovery and understanding of materials with strong spin-orbit effects call for more accurate and scalable electronic structure methods, also capable of operating at finite temperature and dealing with noncrystalline materials.

In this talk, I will first present non-collinear Koopmans-compliant functionals based on densityfunctional perturbation theory [1]. Our theory involves functionals of four-component orbital densities, that are obtained from the charge and spin-vector densities of Wannier functions. I will show numerical simulations for emblematic semiconductors such as GaAs, WSe₂, CsPbBr₃ and the magnetic CrI₃. The predicted band gaps compare well in accuracy to state-of-the-art manybody perturbation theory and include spin-dependent interactions and screening effects that are absent in standard diagrammatic approaches based on the random phase approximation.

Then, I will show how we can probe the local topology of the ground-state electronic structure of non-crystalline and inhomogeneous systems through single-point and space-resolved Z_2 topological markers [2-4]. These topological markers can be deployed both in periodic and open boundary conditions, in presence of disorder and including topological/trivial heterojunctions. Beyond disordered systems, our approach is particularly useful to investigate the role of defects, to study topological alloys and in the context of *ab initio* molecular dynamics simulations at finite temperature.

Finally, I will share first-principles simulations of the temperature effects on the electronic and crystal structure of the 2D topological insulator WTe₂, unravelling the role of thermal expansion, electron-phonon coupling and structural phase transitions in the robustness of its topological phase [5,6].

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16:35-17:05 Alessandro Chiesa (Invited)

MODELING CHIRALITY-INDUCED SPIN SELECTIVITY IN ELECTRON TRANSFER FOR QUANTUM APPLICATIONS

Alessandro Chiesa

Università di Parma, Dipartimento di Scienze Matematiche, Fisiche e Informatiche & Gruppo Collegato di Parma, INFN-Sezione Milano-Bicocca, & UdR Parma, INSTM, Parma, Italy

In the last few years, Chirality-Induced Spin Selectivity (CISS) has been attracting a huge interest, both for its possible role in biological processes and for its exploitation as a powerful technological tool [1]. Electrons transmitted through chiral molecules are highly spin-polarized, even at room temperature and without application of any external magnetic field. The origin of this intriguing effect is still controversial, and stimulates great theoretical efforts to conciliate evidences in very different experimental setups, where the common thread is the presence of a chiral molecule activating the spin selectivity.

In particular, recent observation of CISS in isolated molecules in solution [2] on the one hand paves the way to its exploitation in quantum technologies [3]. On the other hand, such a simplified setup provides also the ideal playground to unravel the origin of CISS.

I will present the first microscopic model of CISS in electron transfer reactions through a chiral molecular bridge [4], in which a photo-excited electron is transmitted from a donor to an acceptor unit, interleaved by a chiral molecule. I will show that a sizable spin polarization can arise from the interplay of coherent and incoherent dynamics, where an essential role is played by strong electron-electron correlations and by the resulting many-body structure of the eigenstates of the chiral molecule. Based on extensive numerical simulations, I will discuss the dependence of this polarization on model parameters and the important role of polarons to potentially amplify the effect. Shedding light on the origin of CISS is the first step towards its technological exploitation. I will present schemes which make use of CISS at the molecular level to initialize, readout or manipulate spin qubits. By working at rather high temperatures (where CISS effect is expected to be highly efficient), this approach can yield remarkable energy savings. Even more notably, by locking spin to charge degrees of freedom, it could give access to the quantum state of individual spins, which is usually hardly accessible due to its weak coupling with external fields.

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17:05-17:20 Federico Orlando (Contributed)

AMaRaNTA: AN AIIDA-BASED WORKFLOW TO AUTOMATE CALCULATIONS OF EXCHANGE PARAMETERS IN 2D MAGNETS

Federico Orlando^{1,2}, Andrea Droghetti², Lorenzo Varrassi³, Srdjan Stavrić², Cesare Franchini^{3,4}, Antimo Marrazzo^{5,6}, Marco Gibertini^{7,8}, Silvia Picozzi²

 Physics Department – Politecnico di Milano, Milan, Italy; 2. Consiglio Nazionale delle Ricerche CNR-SPIN, Chieti, Italy; 3. Dipartimento di Fisica e Astronomia, Università di Bologna, Bologna, Italy; 4. University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria; 5. Dipartimento di Fisica, Università di Trieste, Trieste, Italy; 6. Theory and Simulations of Materials (THEOS) and National Center for Computational Design and Discovery of Novel Materials (MARVEL), École Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; 7. Dipartimento di Scienze Fisiche, Informatiche e Matematiche, Università di Modena e Reggio Emilia, Modena, Italy; 8. Centro S3, Istituto Nanoscienze-CNR, Modena, Italy

2D magnetic materials have sourced great attention in the last few years [1]. Intrinsic theoretical interest arises from the very existence of magnetism below the 3D limit, which has been proven only recently after decades of debate, as well as from the observed richness in magnetic phases, encompassing conventional ferromagnetic and antiferromagnetic as well as more exotic textures. Besides, these materials are known to offer practical applications in fields such as spintronics. The popularity gained by such research field has motivated the adaptation of first-principles approaches, combined with model Hamiltonians, to evaluate exchange parameters, needed for the prediction of magnetic textures [2]. However, the methodology is not uniquely established as of today, which results in a lack of systematicity in the data produced; as a consequence, contrasting predictions may at times arise, preventing a full comprehension of the nature of exchange interaction in some cases [3]. To tackle such issue, we have developed the computational package AMaRaNTA (Automating MAgnetic paRAmeters iN a Tensorial Approach), offering an unprecedented, systematic way of automating Density Functional Theory simulations of exchange parameters for 2D magnets. The output of AMaRaNTA consists of i) the full exchange tensor for 1^{st} nearest neighbours ii) the scalar, isotropic exchange constant for 2^{nd} and 3^{rd} nearest neighbours: both aspects allow us to push the research beyond the state of the art, since previous efforts in this respect were limited to 1st nearest neighbours and non-fully-tensorial approaches only [4]. AMaRaNTA comes in the form of an AiiDA workchain [5], based on the Vienna Ab-initio Simulation Package (VASP) for DFT calculations [6]; actual evaluation of the exchange parameters is done by post-processing DFT total energies via the so-called four-states method [2]. Ease of use is guaranteed in that the user is only required to provide a structure file; AMaRaNTA takes care of building the necessary simulation cells, setting up all calculations, retrieving the results and extracting the exchange parameters.

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17:20-17:50 Jagoda Sławińska (Invited)

SPIN-ORBITRONICS IN CHIRAL CRYSTALS

Jagoda Sławińska

Zernike Institute for Advanced Materials, University of Groningen, Nijenborgh 3, 9747 AG, Groningen, The Netherlands

Chiral materials, similar to human hands, have distinguishable right-handed and left-handed enantiomers which respond differently to external stimuli, such as electric fields. One of the most intriguing aspects of chirality is its impact on charge-to-spin conversion (CSC) which is responsible for transforming electric currents into spin signals. Interestingly, chiral systems often outperform non-chiral ones in terms of conversion efficiency and facilitate long-range spin transport, which makes them relevant for both fundamental and applied physics.

In this talk, I will focus on chiral crystals that manifest chirality-dependent CSC and long-range spin transport. For instance, in different families of chiral materials, represented by Te, FeSi and TaSi2, electric currents induce an accumulation of spins that align either parallel or anti-parallel to them, resembling the phenomenon of chirality-induced spin selectivity (CISS) found in molecules. These materials not only exhibit highly efficient CSC but also possess a so-called quasi-persistent spin texture in reciprocal space, contributing to enhanced spin lifetimes.

ACKNOWLEDGMENTS

I acknowledge the funding from the Dutch Research Council (NWO) under the contract OCENW.M.22.063 and the Rosalind Franklin Fellowship from the University of Groningen.

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17:50-18:20 Andrea Droghetti (Invited)

FIRST-PRINCIPLES ELECTRONIC STRUCTURE AND QUANTUM TRANSPORT METHODS APPLIED TO SPINTRONICS

Andrea Droghetti

CNR-SPIN, Chieti (Italy)

The research field of spintronics focuses on the generation, transport, control, and detection of spin(-polarized) currents in materials and material heterostructures. In this talk, I will present our work on developing theoretical and computational methods to simulate various spintronic systems and effects from first principles. I will begin by reviewing the combination of Density Functional Theory (DFT) with the non-equilibrium Green's functions (NEGF) technique [1]. Specifically, I will explain how we have tailored DFT+NEGF to compute spin(-polarized) currents and out-of-equilibrium magnetic moments [2], with applications ranging from van der Waals [3] to chiral materials [4]. Next, I will describe how DFT+NEGF is further combined with Dynamical Mean Field Theory (DMFT) [5, 6, 7] to address electron correlation beyond a static mean-field level. This method can be applied to spintronic heterostructures, such as Co/Cu/Co or Fe/MgO/Fe, accurately capturing effective mass renormalization and non-coherent effects in the 3d bands of transition metals [8]. Finally, I will describe the extension of this method to study transport beyond the linear response regime, illustrating how electron correlation affects the properties of spintronic systems, such as the 2D ferromagnet Fe₄GeTe₂, when contacted to electrodes and driven out of equilibrium by a bias voltage.

ACKNOWLEDGMENTS

This work began at the School of Physics of Trinity College Dublin (Ireland) with the support of the University Research Fellowship (URF/R1/191769) from the Royal Society and Science Foundation Ireland. It has since continued at CNR-SPIN, funded by the PNRR "National Centre for HPC, Big Data and Quantum Computing" - SPOKE 7.

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Thursday the 28th of August 2024

Surfaces, Interfaces and 2D Materials (9:00-12:50)

9:00-9:50 Carlo Antonio Pignedoli (Keynote)

SIMULATION CHALLENGES IN THE FABRICATION AND CHARACTERIZATION OF QUASI 1D CARBON BASED NANOSTRUCTURES.

Carlo A. Pignedoli

Empa, Swiss Federal Laboratories for Materials Science and Technology, 8600 Dübendorf, Switzerland

The exploration of magnetism in carbon-based nanostructures, particularly through the lens of onsurface synthesis, marks a significant advance in the field of quantum materials. The engineering of many-body quantum states with topological order, utilizing carbon nanomaterials, stands at the forefront of this development, driven by the intrinsic appeal of these materials and their potential as robust platforms for quantum information processing.

This talk will address the simulation challenges related to the electronic and magnetic properties of carbon-based nanostructures [1,2], drawing on research conducted at Empa's nanotech@surfaces laboratory. Additionally, the discussion will connect these challenges to data organization issues in combined experimental and computational research, particularly in the context of advancing towards "automated laboratories".[3]

ACKNOWLEDGMENTS

The work presented was supported by the NCCR MARVEL funded by the Swiss National Science Foundation (Grant No. 205602). The Swiss National Supercomputing Centre (CSCS) is acknowledged for computational resources. PRACE is acknowledged for awarding access to the Fenix Infrastructure resources at CSCS, which are partially funded from the European Union's Horizon 2020 research and innovation program through the ICEI project under the Grant Agreement No. 800858. Also, financial support from the Werner Siemens Foundation (CarboQuant) is greatly appreciated.

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9:50-10:20 Margherita Marsili (Invited)

DEVELOPING TOOLS IN COMPUTATIONAL TRIBOLOGY FOR THE HIGH-THROUGHPUT MODELING OF SOLID-SOLID INTERFACES

Margherita Marsili

Department of Physics and Astronomy, University of Bologna, Viale Carlo Berti Pichat 6/2, Bologna, 40127, Italy

Tribology, the science of interacting surfaces in relative motion, encompasses adhesion, friction, and wear phenomena, which impact a large variety of systems and applications ranging from the nanoscale, where a too strong adhesion might hamper the functioning of nanoelectromechanical devices, to the macroscale where friction coefficients govern the mechanical behavior of earth crust faults. The great challenge of reducing friction makes gaining understanding and developing new lubricant materials even more crucial in view of global emission reduction. Tribology has been traditionally approached by engineering mesoscale methodologies due to the common assumption that only features at that scale mattered. Nevertheless, it is the specific chemistry of the interface that primarily governs adhesion, a measure of the strength by which two surfaces bind together. It also governs the generalized stacking fault energy surface which describes the variation of adhesion between two surfaces as a function of their relative lateral position, ultimately determining the interface resistance to a shear load.

In this framework it is extremely important to develop tools that systematically, and in a highthroughput fashion, determine the intrinsic tribological properties of solid-solid interfaces, including the possible chemical modifications that can affect them from first principles. For this purpose, within the computational tribology group in Bologna, we are developing TribChem [1], a software specifically designed to perform the high-throughput study of solid-solid interfaces. In this work I will introduce the theoretical framework in which Tribchem is developed and, starting from the original version of the code [2], l will give an overview of its current structure, of the general workflow that is implemented, and of the latest developments. I will also show how Tribchem has been applied for the high-throughput determination of the adhesion energy and of the tribological properties of metal-metal [3] and metal-semiconductor heterostructures.

ACKNOWLEDGMENTS

These results are part of the SLIDE project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant agreement No. 865633).

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TRANSPORT PROPERTIES OF SOLID-STATE ELECTROLYTES AT HYBRID DFT-LEVEL WITH MACHINE LEARNING

Davide Tisi

Laboratory of Computational Science and Modeling, Institut des Matériaux, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

Lithium ortho-thiophosphate (Li₃PS₄) is a promising solid-state electrolyte for batteries, yet the microscopic mechanisms governing Li-ion transport within it remain unclear. Moreover, no computational work has computed the thermal conductivity at the DFT level. In this talk, I will show how we build machine learning potentials trained over state-of-the-art DFT references (PBEsol, SCAN, and PBE0), to study the electrical [1] and thermal conductivity [2] of all the known phases of Li₃PS₄ (α , β and γ), for large system sizes and timescales. I will discuss the physical origin of the observed superionic behaviour of Li₃PS₄: where the the PS₄ flipping drives a structural phase transition to a highly conductive phase, characterised by an enhancement of Li-site availability and by a drastic reduction in the activation energy of Li-ion diffusion. I will show the effect of the phase transition on both the electrical and thermal conductivity. We elucidate the role of inter-ionic dynamical correlations in charge transport by highlighting the failure of the Nernst-Einstein approximation to estimate the electrical conductivity. Finally, we will discuss how thermal conductivity presents two distinct behaviours: low and constant with temperature for the α and β phases, and a phonon-like behaviour for the γ phase.

ACKNOWLEDGMENTS

We acknowledge funding from: the Swiss National Science Foundation (SNSF) under the Sinergia project CRSII5_202296, MARVEL National Centre of Competence in Research (NCCR) for computational resources and European Research Council (ERC) under the European Union's Horizon 2020 research and innovation programme Grant No. 101001890-FIAMMA.

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11:20-11:50 Silvia Bonfanti (Invited)

MACHINE LEARNING DISCOVERY IN HIGH ENTROPY MATERIALS: DERIVATIVES OF CANTOR ALLOYS AND COMPLEX GLASSES

Silvia Bonfanti

Center for Complexity and Biosystems, Department of Physics "Aldo Pontremoli", University of Milan, Via Celoria 16, 20133 Milano, Italy

High entropy materials, including alloys (HEAs) and metallic glasses (HEMGs), are at the forefront of materials science due to their exceptional properties derived from compositional complexity. This work employs machine learning (ML) to uncover and refine the properties of these materials, demonstrating significant advancements in HEAs and initiating the exploration of HEMGs.

For HEAs, we applied Bayesian optimization with compositional constraints, enhancing the mechanical properties of the Cantor alloy and discovering compositions like Fe21Cr20Mn5Co20Ni34 and Fe6Cr22Mn5Co32Ni35, which show in silico marked improvements in "single crystal" yield stress [1]. This success showcases the potential of ML in optimizing the complex compositional landscape of HEAs and paves the way for the design of several material properties simultaneously.

The brittleness and ductility of metallic glasses are of high interest. Extending this methodology to HEMGs, we will show results on the optimization of the mechanical properties in this regard. Although in the early stage, our results pave the way for applying high entropy concepts to disordered materials.

Our ML-driven approach enhances HEAs and gives the basis for innovative advancements in HEMGs, showcasing the potential of ML and Bayesian methods in the discovery and optimization of high entropy materials for diverse applications.

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11:50-12:05 Andrea Corradini (Contributed)

A MACHINE LEARNING APPROACH TO LIGHT-INDUCED ORDER-DISORDER PHASE TARNSITIONS: LARGE-SCALE LONG-TIME SIMULATIONS WITH *AB INITIO* ACCURACY

Andrea Corradini, Giovanni Marini, Matteo Calandra

Department of Physics, University of Trento, 38123 Povo, Italy

While machine learning has excelled in simulating material thermal properties, its application to light-induced order-disorder non-thermal phase transitions has been limited by challenges in accurately describing the potential energy surface, the forces and the vibrational properties in the presence of a photoexcited electron-hole plasma. Here, we present a novel approach that combines constrained density functional perturbation theory [1] with machine learning techniques, yielding highly reliable interatomic potentials capable of capturing electron-hole plasma effects on structural properties. Applied to photoexcited silicon, our potential is ten times more accurate than previous models [2]. We show that, at low enough temperatures, the non-thermal melting transition is driven by a soft phonon and the formation of a double well potential, at odds with thermal melting being strictly first order. Our method paves the way to large-scale long-time simulations of light-induced order-disorder phase transitions in materials with ab initio accuracy.

ACKNOWLEDGMENTS

These results are part of the "Discovering light induced phases by first principles materials design (DELIGHT)" project that has received funding from the European Research Council (ERC) under the European Union's Horizon Europe research and innovation program (Grant agreement No. 101052708). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them.

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12:05-12:20 Ivan Rivalta (Contributed)

MODELING OF GOLD NANOBIPYRAMIDS: FROM ANISOTROPIC GROWTH TO CHIRAL PROPERTIES

Ivan Rivalta

Università degli Studi di Bologna, Dipartimento di Chimica Industriale "Toso Montanari", Via Piero Gobetti 85, I-40129 Bologna, Italy

The great and tunable plasmonic properties of gold nanobipyramids (AuBPs), superior for instance to those of gold nanorods, make them highly effective for many applications, including sensing and catalysis. In this presentation, I will illustrate our latest advancements in computational modeling of AuBPs [1-3]. Our results provide insights into the critical role of surfactants in the anisotropic growth of AuBPs, enabling the formation of monodisperse structures with exceptional optical characteristics. We simulated the plasmonic response of various AuBPs and compared different methodologies (discrete dipole approximation, boundary element methods and quasistatic approximation) aiming for a reliable approach to simulate the electronic coupling with molecular chromophores in nano-hybrid systems. Additionally, we examined how AuBPs can serve as versatile templates for creating multi-metallic composites with tunable shape and peculiar optical properties. In particular, we investigated Au@Ag and Au@Au nanoparticles designed to achieve intense plasmonic circular dichroism. Combined experimental and computational results highlighted the key role played by the nanoparticles' surface on the chiral properties. Finally, recent results revealing the role of molecular chiral encoders on the formation of the chiral surfaces and the presence of chiral-induced aggregation in AuBPs aggregates are presented.



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EXPLORING ATOMIC DYNAMICS IN METALS WITH MOLECULAR DYNAMICS AND MACHINE LEARNING

Massimo Delle Piane; Matteo Cioni; Mattia Perrone; Giovanni M. Pavan

Department of Applied Science and Technology, Politecnico di Torino, Torino, Italy

Understanding the atomic-scale dynamics of metal surfaces is crucial for advancements in catalysis, nanoelectronics, and materials science. This presentation delves into the complexities of atomic movements on metal surfaces through an advanced analysis that integrates machine learning (ML) with molecular dynamics (MD) simulations.

By employing advanced descriptors such as the Smooth Overlap of Atomic Positions (SOAP) and its temporal variant TimeSOAP (tSOAP),[1] along with the Local Environments and Neighbors Shuffling (LENS) framework,[2] we achieve precise characterization of atomic environments in high-dimensional data from MD simulations. These methodologies enable us to identify dynamic domains and uncover the "statistical identities" of atoms within gold nanoparticles[3-4] and copper surfaces,[5] providing new insights into their hidden dynamics. Our research challenges the conventional perception of metals as static, rigid materials by revealing the dynamic nature of atoms on their surfaces. The integration of ML techniques discerns the complex interplay of atomic environments, which is vital for predicting the behavior of metal surfaces under various conditions, including catalytic processes and mechanical stress scenarios involving dislocations and fracture. Moreover, combining experimental techniques, such as annular dark-field scanning transmission electron microscopy (ADF-STEM), with advanced computational methods, we overcome the limitations of traditional experimental and simulation approaches.[4]

This integration offers a novel perspective on the atomic-scale dynamics of metal surfaces. Our findings highlight the fundamental role of atomic dynamics in defining the properties of metals, paving the way for future innovations in material science.

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Quantum Science and Technologies (14:10-18:15)

14:10-15:00 Simone Montangero (Keynote)

TENSOR NETWORK ALGORITHMS FOR HIGH-DIMENSIONAL QUANTUM MANY-BODY SYSTEMS

Simone Montangero

Università di Padova, Italia

We review some recent results on the development of efficient tree tensor network algorithms and their applications to high-dimensional many-body quantum systems. In particular, we present results on two- and three-dimensional systems including two dimensional Rydberg atom systems, and lattice gauge theories in presence of fermonic matter and to the computation of the entanglement of formation in critical many-body quantum systems at finite temperature. Finally, we present the application of tensor network methods to the solution of hard classical combinatorial problems via mapping to many-body quantum hamiltonians. 15:00-15:15 Chiara Capecci (Contributed)

PULSE – VARIATIONAL QUANTUM EIGENSOLVER

Daniel J. Egger¹, Chiara Capecci², Bibek Pokharel³, Panagiotis Kl. Barkoutsos¹, Laurin E. Fischer^{2,4}, Leonardo Guidoni⁵, Ivano Tavernelli¹

 IBM Quantum - IBM Research Europe - Zurich, Switzerland; 2 Dipartimento di Ingegneria e Scienze dell'Informazione e Matematica, Università degli Studi dell'Aquila, L'Aquila, Italy – currently: Dipartimento di Fisica, Università di Trento, Trento, Italy; 3 IBM Quantum – IBM Research Almaden, San José, California, USA; 4 Theory and Simulation of Materials (THEOS), Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland; 5 Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy

State-of-the-art noisy digital quantum computers are currently limited to executing short- depth quantum circuits. Variational algorithms offer a promising solution for exploiting the potential of these noisy quantum systems, as they can operate within the hardware's depth constraints [1,2]. In our work, we propose encoding the variational parameters directly as hardware pulse amplitudes and durations [3]. This approach significantly shortens the pulse schedule and overall circuit duration, thereby mitigating the effects of qubit decoherence and gate noise [4]. We demonstrate the effectiveness of our Pulse-Variational Quantum Eigensolver (Pulse-VQE) algorithm by calculating the ground state of hydrogen-based systems (H2, H3, and H#) using IBM's cross-resonance-based hardware [5]. Our method achieves a schedule duration reduction of up to $5\times$ compared to CNOT-based Ansätze and lower measured energy. Notably, we observe a substantial improvement in the minimal energy configuration of H3 with our pulse-based approach compared to CNOT-based variational form.



Figure: Optimized pulse schedules for H2 at 0,2 Å. (a) CNOT-based and (b) pulse-based Ansätze. The circular arrows indicate zero-duration virtual-Z gates (VZ). The drive channels D\$ indicate single-qubit pulses on qubit i and the control channels U\$ indicate cross- resonance tones.

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15:15-15:45 Elisa Ercolessi (Invited)

HYBRID VARIATIONAL ALGORITHMS ON A NEUTRAL ATOM PLATFORM

Elisa Ercolessi

Department of Physics and Astronomy – University of Bologna INFN-Sezione di Bologna

Quantum Computing is seen as a potential breakthrough for the study of hard classical problems as well as for quantum many body systems. However, we are in the era of NISQ devices and still far away from fault-tolerant machines.

This leads us to consider the possibility of hybrid classical-quantum protocols of variational type: they exploit quantum resources to efficiently prepare states that depend on a suitable chosen set of variational parameters, which can then be determined by means of optimization algorithms to be run on a classical computer. The choice of such classical optimizer schemes is to be guided by compatibility requirements with respect to current available quantum platforms.

To evaluate the feasibility of such an approach, we present an application of the Quantum Approximate Optimization Algorithm to a typical classical hard combinatorial problem, that has been emulated and tested on the Rydberg atom quantum machine Fresnel of Pasqal.

SIMULATING SPIN DEFECTS IN SOLIDS FOR QUANTUM TECHNOLOGIES

Marco Govoni

University of Modena and Reggio Emilia, Via Campi 213/a, Modena, Italy

Electrons bound by a point-defect to a region on the order of a single lattice constant can be regarded as analogues of atomic systems in an effective vacuum, with spin and optical properties that are determined by the interplay between the defect and the host material. Prototypical examples of this are the NV-centers in diamond. We present theoretical and computational resources to accelerate the development of spin-defects as solid-state qubits with robust quantum characteristics for applications in quantum sensing, quantum communications, and quantum computing. We focus on the calculation of photoluminescence spectra of defects which require an accurate description of atomic displacements in electronic excited states. For this purpose, we use a hierarchical modeling approach that relies on the combination of time-dependent density functional theory (TDDFT), many-body perturbation theory (GW/BSE), and multi-reference methods. We discuss a formulation of spin-conserving and spin-flip TDDFT, including the calculation of forces in excited states, and a computational framework to carry out electronic structure calculations of solids using embedded Green's function theory. These examples benefit from the use of the latest developments in high-performance computing architectures, which include pre-exascale capable machines and quantum processors. Although applications of quantum computing to condensed matter physics are in their infancy, we show that promising results for realistic systems appear to be within reach combining zero-noise extrapolation techniques and symmetry-constraining ansätze.

16:45-17:15 Leonardo Fallani (Invited)

STRONGLY INTERACTING LATTICE FERMIONS: FLAVOUR-DEPENDENT MOTT LOCALIZATION AND UNIVERSAL HALL RESPONSE

Leonardo Fallani

Dipartimento di Fisica e Astronomia, Università degli Studi di Firenze LENS & CNR-INO, Sesto Fiorentino (FI), Italy

I will present the results of recent experiments performed with ultracold ¹⁷³Yb fermions in optical lattices, in the presence of strong atom-atom interactions and coherent driving between different internal states.

I will discuss the realization of interacting SU(N) Fermi-Hubbard systems, where the addition of a coherent Raman coupling between different spin states is used to induce a controlled breaking of the SU(N) global interaction symmetry. This explicit symmetry-breaking action is shown to favour Mott localization and determines the onset of a flavour-selective behavior [1], in connection with the physics arising in strongly correlated materials from the coupling of different orbitals.

I will also discuss recent experiments where we have measured the Hall conductivity in interacting synthetic ladders obtained from a momentum-dependent Raman coupling, which implements the action of an external magnetic field on effectively charged particles. I will show a strong dependence of the Hall response upon changing atom-atom interactions and the emergence of a universal regime in the strongly interacting limit [2]. I will then discuss recent developments with the measurement of Hall voltages and Hall resistances, which provide a direct connection between quantum simulations and the most common measurements in solid-state systems.

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17:15-17:45 Matteo Michele Wauters (Contributed)

ANALOG QUANTUM SIMULATIONS OF MANYBODY SYSTEMS WITH TUNABLEJOSEPHSON JUNCTION ARRAYS

Matteo Michele Wauters

Pitaevskii BEC Center, Department of Physics, University of Trento, Trento, Italy INFN-TIFPA, Trento Institute for Fundamental Physics and Applications, Trento, Italy

The development of Josephson junction arrays (JJA) based on hybrid superconductor – semiconductor devices allows for a remarkable level of control of their main physical parameters [1]. This makes them appealing platform for engineering and simulating quantum many-body physics [2-4], in particular for transport properties as JJAs are easily interfaced with both metallic and superconducting leads. Here, we focus on a particular design for a one-dimensional JJA where the building blocks can be tuned into a phase with symmetry, each realizing an effective "qutrit"[4]. By controlling the charging energies of the superconducting islands and their Josephson couplings, we investigate its potential as an analog quantum simulation platform for quantum clock models. Through matrix-product states simulations, we explore their rich phase diagram, and suggest which experimental observables can be adopted in realistic devices to probe the physics and the phase transitions of the model.



Figure 1: sketch of the proposed platform for analog quantum simulations of the clock model

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17:45-18:15 Luca Barbiero (Invited)

EXPLORING STRONGLY INTERACTING FERMIONIC QUANTUM MATTER WITH MAGNETIC ATOMS

Luca Barbiero

Institute for Condensed Matter Physics and Complex Systems, DISAT, Politecnico di Torino, I-10129 Torino, Italy

Strongly interacting fermions in a reduced dimensionality are a key playground for unveiling fascinating states of matter. In this regard, superconductivity and topologiy represent paradigmatic examples. In this talk, I will show that ultracold magnetic atoms trapped in optical lattice could enable an in depth investigation of these quantum phases. The exceptional versatility offered by this types of particles, makes it indeed possible to design many-body Hamiltonians in the form of generalized t-J models, in which tunable long-range magnetic couplings compete with the onsite interaction and the tunneling processes. Through analytical and numerical analysis, our results demonstrate such complexity to be the responsible for the appearance of a rich phase diagram characterized by different superconducting and symmetry protected topological phases. Notably, these states of matter take place in experimentally accessible regimes and can be probed with standard measurement schemes thus showing the importance of magnetic atoms for a deeper comprehension of strongly interacting quantum matter.

ACKNOWLEDGMENTS

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REFERENCES L. Bellinato Giacomelli, T. Bland, L. Lafforgue, F. Claude, F. Ferlaino, M. Mark, L. Barbiero in preparation Friday the 30th of August 2024

Statistical Mechanics and emergent phenomena (9:00-12:50)

9:00-9:50 Amos Maritan (Keynote)

OPTIMALITY AND SCALING IN PLANTS AND FORESTS

Amos Maritan

Department of Physics and Astronomy – University of Padova – Italy

Living systems exhibit recurring patterns and regularities that transcend their biological and physiological specifics. These phenomena often manifest as approximate power-law distributions and long-range correlations, observable at both the individual and community levels. Understanding how general trends and behaviors emerge, and how individual traits scale to influence community assembly, remains a significant challenge. In this talk, we begin with a variational principle that predicts the geometry and scaling of xylem structures, the conduits responsible for water transport from roots to leaves. We then extend this analysis to the scaling properties of entire plants and natural plant communities, specifically forests. Forests, characterized by their structural and functional diversity, represent one of the most complex systems in nature. Despite this complexity, we uncover a remarkable simplicity underlying forest dynamic. Our approach is grounded in optimization and variational principles, enabling predictions of body mass-metabolic scaling, size distributions within plant communities, and pair correlation functions versus distance. These predictions are rigorously tested across forests at various latitudes. Deviations from the predicted models are used to quantify the extent of ecological disturbances. This talk will highlight how theoretical principles can elucidate the intricate yet fundamentally simple rules governing complex biological systems, with a focus on forests as a model system.

VARIANCE SUM RULE(S) FOR ENTROPY PRODUCTION

Ivan Di Terlizzi

Max Planck Institute for the Physics of Complex Systems, Dresden

Non-equilibrium steady states, from the planetary scale to biological processes, are characterized by entropy production via energy dissipation to the environment, which is often challenging to measure. We introduce a variance sum rule (VSR) for displacement and impulse variances that permits us to measure the entropy production rate σ in nonequilibrium steady states. We first illustrate it for directly measurable forces, such as an active Brownian particle in an optical trap. By further introducing a model-dependent fitting procedure, we develop a method based on the VSR to derive σ from one-dimensional stochastic traces without measuring forces. In particular, we apply this inference procedure to flickering experiments in human red blood cells. We find that σ is spatially heterogeneous with a finite correlation length, and its average value agrees with calorimetry measurements.

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Variance Sum Rule for Entropy Production, I. Di Terlizzi et al., Science 383 (2024) Variance Sum Rule: proofs and solvable models, I. Di Terlizzi et al., New Journal of Physics (2024)

CONTROLLING FLOW PATTERNS AND TOPOLOGY IN ACTIVE EMULSIONS

Giuseppe Negro

Università degli studi di Bari "A. Moro", Dipartimento Interateneo di fisica "M.Merlin"

Active nematics are a class of liquid crystals composed of rod-like constituents that convert energy from their surroundings to exert mechanical forces that intrinsically drive the material out of equilibrium[1]. These materials display spontaneous disorderly flows and a steady-state populations of topological defects through continuous pair creation and annihilation. Studies have found complex dynamical behaviors associated to defects[2] —including self-propulsion in two dimensions, and defect loop formation and growth in three dimensions[2]. Understanding how defect dynamics relate to the emergent flows and how to control these non-equilibrium states is an ongoing topic of research. In this talk we present results regarding the morphology and spatiotemporal dynamics of active emulsions, where one or two passive small droplets are embedded in a larger active droplet. We find that activity introduces a variety of rich and nontrivial non-equilibrium states in the system, while the different topological configurations can be tuned by changing the number of passive inner cores[3]. These emulsions can be self-assembled in the lab and provide a pathway to form flow and topology patterns in active matter in a controllable way, as opposed to bulk systems that typically yield active turbulence.

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SIMULATING REACTIONS AT SLIDING INTERFACES BY AB INITIO AND MACHINE LEARNING MOLECULAR DYNAMICS

Paolo Restuccia, Mauro Ferrario, M. Clelia Righi

Dipartimento di Fisica e Astronomia, Università di Bologna, Bologna, Italy

Tribological phenomena, such as wear and boundary lubrication, are deeply influenced by tribochemical reactions, which are chemical reactions occurring at the interface of two bodies in contact in the presence of mechanical stresses. It is extremely difficult to monitor these phenomena in real time by experiments. Computational approaches represent an invaluable tool to understand the microscopic mechanisms of friction and wear and provide their atomistic description. In particular ab initio molecular dynamics (MD), which allows for an accurate description of chemical reactions occurring in conditions of enhanced reactivity as the tribological conditions [1–3]. For example, we fully unraveled how molybdenum dithiocarbamate, a common lubricant additive, transforms into molybdenum disulfide crystal due to mechanical stresses with ab initio calculations [1]. These stresses synergise in rearranging the amorphous units into a crystalline structure by overcoming the energy barriers associated with the bond formation. However, the high computational costs associated with the use of ab initio MD, limits time scale and size of the simulated systems. To overcome these limitations, while maintaining the same 'quantum' accuracy, we adopted machine learning interaction potentials generated by employing a workflow for active learning linked to Quantum Espresso developed by our group, and tested for tribological applications [4,5]. Here, we apply this tool to for simulating the tribochemical reactions involving organophosforus additives for engine oils [6] a prototypical system composed by methyl thiolate molecules confined between a copper interface, which is analysed by complementary Atomic Force Microscopy experiments. By comparing the computational and experimental results for reaction rates and pathways we derive fundamental understanding on the kinetics of chemical reactions activated by mechanical forces within the framework of Evans and Polanyi theory [7].

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These results are part of the "Advancing Solid Interface and Lubricants by First Principles Material Design (SLIDE)" project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant agreement No. 865633).

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11:35-12:05 Vittoria Sposini (Invited)

BEING HETEROGENOUS IS ADVANTAGEOUS: EXTREME BROWNIAN NON-GAUSSIAN SEARCHES

Vittoria Sposini

Dipartimento di Fisica e Astronomia 'G. Galilei', Università di Padova, Via Marzolo 8, 35131 Padova (PD), Italy.

Redundancy in biology may be explained by the need to optimise extreme searching processes, where one or few among many particles are requested to reach the target like in human fertilisation. In this talk I will show that non-Gaussian rare fluctuations in Brownian diffusion dominates such searches, introducing drastic corrections to the known Gaussian behaviour. In particular, starting from a subordination approach I will study different models such as diffusing diffusivity models, polymers in the grand canonical ensemble, and polydisperse polymers, all exhibiting stages of non-Gaussian diffusion. The origin of non-Gaussianity is amenable to the heterogeneity of the ensemble of diffusers and/or of the environment. Such heterogeneity implies both an excess of probability in the central part and in the tails of the displacements distribution, when compared with the Gaussian one (Figure 1). I will show that a higher probability for few, faster diffusers (tail effect) influences extreme searches, pointing out that a redundant information stored in diverse searchers strongly enhances the fast targeting of the first few instances.



Figure 1: Comparison between Gaussian and non-Gaussian probability density functions (PDFs) for subordination processes. The two PDFs share the same mean and standard deviation but the non-Gaussian one has an excess probability both in the tails and in the center part.

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12:05-12:35 Maria Chiara Angelini (Invited)

A NEW RENORMALIZATION GROUP APPROACH TO DISORDERED SYSTEMS

Maria Chiara Angelini

Dipartimento di Fisica, Università di Roma La Sapienza, Roma, Italy

The renormalization group (RG) approach is a standard method to characterize second order phase-transitions. In standard RG, one aims to find the solution of a model in finite-dimensions expanding around the mean-field fully connected (FC) solution. However, this approach has some problems when applied to disordered systems: the main reason is that in the FC models no fluctuations in the fields are present and local observables converge to global ones. I will show how to introduce a new expansion, for which the starting point is a different soluble MF model: the Bethe lattice (BL) model. At variance with the FC one, this model shares a crucial property with finite-dimensional models: the finite connectivity of the lattice. Its inclusion is essential because it implies the local fluctuations of important observables and allows us to describe heterogeneity. I will then show the results of the application of this new expansion to many disordered models: (random field) Ising model, percolation model and spin-glass model.

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ABSTRACTS OF POSTERS

Session 1 – Wednesday the 28th of August 2024 – 18:30-19:30

Nicolas Baù	Theory of local Z2 topological markers for finite and periodic systems
Davide Bidoggia	Structural phase transition in monolayer TMDs from neural-network molecular dynamics
Alberto Bottarelli	Qudit for Quantum optimization
Pietro Nicolò Brangi	Tunable magnetism and half metallicity in field-effect doped 2d graphitic carbon nitride
Luigi Camerano	Magneto-orbital coupling in vanadium trihalides
Alessio Cucciari	NbTi: a nontrivial puzzle for the conventional theory of superconductivity
Elisa Damiani	Rationalizing the role of surface chemical modifications to tune interface adhesion
Paolo Fachin	Quantized Born Effective charges as probes for the topological phase transition in the Haldane and Kane-Mele models
Mauro Ferrario	Molecular dynamics simulation of eco-friendly lubricant additives
Vito Foderà	Designing optimal catalyst for hydrogen and carbon nanotube production via methane pyrolysis
Pietro Maria Forcella	Pressure induced superconductivity in HgS

THEORY OF LOCAL Z2 TOPOLOGICAL MARKERS FOR FINITE AND PERIODIC SYSTEMS

Nicolas Baù¹ and Antimo Marrazzo²

¹ Dipartimento di Fisica, Università di Trieste, Trieste, Italy ² Scuola Internazionale Superiore di Studi Avanzati (SISSA), Trieste, Italy

Topological invariants are global properties of the ground-state wave function, typically defined as winding numbers in reciprocal space. Over the years, a number of topological markers have been introduced, allowing to probe the topological order locally in real space even for disordered and inhomogeneous systems [1]. Here, I will address time-reversal symmetric systems in two dimensions and introduce two local Z2 topological markers [2]. The first formulation is based on a generalization of the spin-Chern number [3] while the second one is based solely on time-reversal symmetry [4]. Then, I will introduce a formulation of the local Chern marker for extended systems with periodic boundary conditions [5, 6], and I extend it to the aforementioned Z2 markers [7]. Finally, I will show numerical simulations to validate the approach, including pristine disordered and inhomogeneous systems, such as topological/trivial heterojunctions.

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STRUCTURAL PHASE TRANSITION IN MONOLAYER TMDS FROM NEURAL-NETWORK MOLECULAR DYNAMICS

Davide Bidoggia, Riccardo Dal Molin, Leonid Kahle, Maria Peressi, Antimo Marrazzo

Università di Trieste, Italia

Among the wide family of layered materials, transition metal dichalcogenides (TMDs) constitute a broad class of systems exhibiting diverse properties depending on chemical composition, temperature, pressure, and dimensionality.

In the single layer limit, some TMDs can exhibit different polymorphs, as for instance tungsten ditelluride (WTe2) and molybdenum ditelluride (MoTe2) which showcase two dynamically stable phases characterized by a small energy.

Here, we develop neural-network interatomic potentials trained on density-functional theory and investigate at the atomistic level the structural transition between the two polymorphs. Although the phases are close in energy, they are separated by a large energy barrier and possibly complex transition pathways. By performing molecular dynamics simulations, we examine the role of defects and interfaces in driving the structural change from the metastable to the most stable phase at high temperature.

TUNABLE MAGNETISM AND HALF METALLICITY IN FIELD-EFFECT DOPED 2D GRAPHITIC CARBON NITRIDE

Pietro Nicolò Brangi

Department of Physics, University of Trento, Italy

Graphitic carbon nitride $(g-C_3N_4)$ has sparked a lot of interest for its notable photocatalytic and photoelectronic properties [1] that are reported in many works, both theoretical and experimental, even though its structural and electronic features are not yet fully understood.

One of the most interesting features of the material is the presence of a very flat valence band over the whole Brillouin zone. Such an electronic structure, due to the lone pairs localized on the nitrogen atoms, raises the question of whether correlated states can be stabilized upon doping.

In our work we first shed light on the ground state atomic structure of monolayered g- C_3N_4 , which, following the work reported in [2], we show to be a $\sqrt{3} \times \sqrt{3} R 30^\circ$ supercell, corrugated as in fig.1. Furthermore, we study the dynamic stability of such structure calculating its phonon dispersion, thus proving that the supercell we are considering corresponds to the ground state.

We then investigate the properties of the material as a function of the doping, in a Field Effect Transistor setup, finding that even a small amount of charge leads to the stabilization of a half-metallic state, with the spin polarized charges localized on the nitrogen atoms' lone pairs (fig.2b). The material then displays a rich behavior, going from a half-metal to an insulator back to a half-metal, as the doping increases, with the magnetization of the monolayer reaching large values up to several μ^{B} 's (fig.2a). Our work thus paves the way for a more complete understanding of graphitic carbon nitride in photocatalytic cells, where the material is subject to electric fields, and for a possible application of g- C₃N₄ in the field of spintronics as a 2D tunable half metal.



Fig. 1: optimized $\sqrt{3} \times \sqrt{3} R30^{\circ}$ supercell of g- C₃N₄. One can notice the large corrugation and distortion of the heptazine units.

Fig. 2: (a) magnetization of the monolayer as a function of the doping; (b) spin polarized charge density of g- C_3N_4 doped with 1.5 holes/unit cell

ACKNOWLEDGMENTS

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MAGNETO-ORBITAL COUPLING IN VANADIUM TRIHALIDES

Luigi Camerano¹, A. O. Fumega, G. Profeta, J. L. Lado

¹Department of Physical and Chemical Sciences, University of L'Aquila, Via Vetoio, 67100 L'Aquila, Italy

Strongly localized electrons on the specific atomic sites are characterized by charge, spin and orbital degrees of freedom which in some cases could be coupled giving rise to various functional properties such as ferroelectricity, multiferroicity, superconductivity and altermagnetism [1-4]. The presence of multiorbital degeneracy represents a powerful playgroup to display entangled electronic orders [5]. Indeed, the fundamental ingredient to realize spin-orbital entangled Hamiltonian in real systems is the presence of strongly correlated electrons in a degenerate manifold. By means of first principle calculations [6,7], we establish the presence of magneto-orbital coupling in the 2D magnets vanadium trihalide VCl₃ proposing an ab-initio mapping onto a spin and pseudo-spin Hamiltonian (see Figure). We establish the coupling between orbital and magnetic degrees of freedom, unveiling the emergence of hybrid magnon-orbital excitations [7]. Our results establish VCl₃ as a promising 2D material to observe emergent magneto-orbital excitations and providing a platform for multicomponent symmetry breaking.



(a) schematic representation of the V-d orbitals in an octahedral environment (O_h) and two possible electronic configurations after trigonal distortion (D_{3d}). The corresponding DFT+U density of state projected on V-d is reported in the lower panel showing orbital order states. (b) calculated magnetization density $(n\uparrow - n\downarrow)$ in the case of ferromagnetic ferro-orbital (C_{2h} symmetry) and ferromagnetic antiferro-orbital (C_{1h} symmetry). (c) Sketch of the model presented: the distinct colours for the orbitals highlight different V-sites in the antiferro-orbital phase.

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NBTI: A NONTRIVIAL PUZZLE FOR THE CONVENTIONAL THEORY OF SUPERCONDUCTIVITY

Alessio Cucciari, Dionisia Naddeo, Simone Di Cataldo and Lilia Boeri

Dipartimento di Fisica, Sapienza - Università di Roma, Rome, Italy Dip. di Biomedicina e Prevenzione, Università degli Studi di Roma Tor Vergata, Rome, Italy

In this paper we present the first *ab-initio* study of the superconducting state of NbTi, traditionally considered the main workhorse for many large-scale superconducting applications. Despite being a "textbook" material, this compound represents a major challenge for current computational standards in superconductivity. Using the newly developed SSCHA-MLIP framework, we demonstrate that anharmonic effects are required to obtain stable phonon dispersions for the ordered bcc phase, which is unstable at the harmonic level. We also find that treating the residual Coulomb interaction in the newly-developed Kukkonen-Overhauser scheme reduces the T_c by more than 20% compared to the simple Morel-Anderson approximation. We show that the unusually large residual discrepancy in T_c with respect to experiment should be attributed to lattice

disorder, which we treat with a simple model of Boltzmann-averaged supercells. Our results indicate that a quantitative description of technologically-relevant transition metal alloy superconductors requires methodological developments to account for lattice disorder that go beyond the current standards in computational superconductivity.



Fig. 1. a) electronic band structure of β -NbTi. The inset shows the Fermi surface, with different colors denoting different bands. b) Atom-projected density of states (DOS) in units of states/eV/at. Projections onto Nb and Ti are shown in orange and blue, respectively. The zero of the energy is the Fermi level. c) In this panel, the DOS of the ordered phase is compared with that of a simple model of a disordered phase

Fig. 2. a) anharmonic (full black lines) phonon dispersions of the ordered β -NbTi, decorated with their linewidths (red shading). The corresponding harmonic phonons are represented by dashed black lines. The inset shows the vibration pattern of one of the two unstable eigenmodes at the M point. b) Atom-projected and total phonon density of states in units of states/meV. c) Atom-projected and total Eliashberg spectral function, along with the electron-phonon coupling $\lambda(\omega)$ (dotdashed black line) d) Nesting function $\eta(0)(\mathbf{q})$. Red arrows highlight the position of Kohn anomalies. e) Projection of the Fermi surface onto the [110] lattice plane; black arrows indicate parts of the Fermi surface which contribute to the peak in the nesting functions for $\mathbf{q} = \mathbf{M}$.

Fig. 3. Energy distribution of the zero-frequency superconducting gap of ordered β -NbTi as a function of temperature, obtained solving the anisotropic Migdal–Eliashberg equations for $\mu * = 0.20$. The distribution of the superconducting gap over the Fermi surface is reported in the inset with a color scale which goes from the minimum to the maximum value of the gap (4.5 to 5.8 meV). Dashed lines indicate a fit of the weighted averages of the distribution for each T in red, the corresponding isotropic solution in black, and the isotropic solution for the disordered model in blue.

The authors would like to thank C.Heil, R. Lucrezi, E. Kogler for help with the SSCHA-MLIP calculations, and A. Sanna for discussion and for performing the calculations of the Coulomb interaction beyond the μ * approximation. We would also like to thank Alex Gurevich and David Larbastier for useful discussion on NbTi literature.

RATIONALIZING THE ROLE OF SURFACE CHEMICAL MODIFICATIONS TO TUNE INTERFACE ADHESION

Elisa Damiani, Margherita Marsili and Maria Clelia Righi

Department of Physics and Astronomy "Augusto Righi", University of Bologna (Italy)

Diamond and diamond-like carbon (DLC) coatings represent an important class of solid lubricants that, exploiting the outstanding properties of diamond, provide some of the lowest known friction coefficients and wear rates [1] [2]. For these reasons, they are largely used in industry to reduce friction and wear in engine components, to avoid stiction in micro- and nano-electromechanical systems (NEMS and MEMS) and to increase the longevity and functionality of biological implants and industrial cutting tools [3] [4]. A significant limitation in their employment concerns their spallation from the substrate [5] [6]; on the other hand, to reduce friction, quenching the adhesion

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with any countersurface would be highly desirable [7]. It is thus interesting to explore how DLCs adhesion can be tuned through chemical modifications of its surfaces. We employed ab initio simulations to study the effect of surface reconstruction and chemical species intercalation (B, P, O, F, N, S, H) on the adhesion of non-reconstructed and Pandey-reconstructed C(111)/Cu(111) interfaces to identify the basic mechanisms at play when the interaction between the two surfaces is either enhanced or quenched. We found that the increment of graphitization at the diamond surface decreases the adhesion, associated with a less amount of electronic charge accumulation at the interface region. Moreover, when a high degree of surface graphitization is present the best way to increase adhesion is to select atoms able to act as chemical bridges (e.g., B and N), compensating for the lack of interaction between the surfaces. Conversely, adhesion reduction of $\sim 100\%$ can be achieved, regardless of the degree of surface graphitization, by intercalating an atomic species that does not bond with the countersurface and prevents the interaction between the slabs, i.e. F and S. This study highlighted the outstanding and universal properties of fluorine in reducing adhesion. Motivated by these findings, we further examined the mechanisms underlying this effectiveness to identify the physical reason behind it. With this objective, we investigated by means of density functional theory calculations two representative sets of systems, PTFE and fluorinated diamond in contact with metallic surfaces. By comparing the role of F and H terminations we demonstrated that the lubricant effect of fluorine species is primarily due to its strong Pauli repulsion with the counter surfaces. This interaction, of quantum mechanical origin, makes the atoms with filled electronic shells behave as hard spheres that interact through high repulsive forces when come into contact, because they cannot interpenetrate each other. This leads to the increment of the interfacial distance between any kind of countersurface, thus reducing interface adhesion and friction. Our findings suggest a universal lubrication mechanism driven by Pauli repulsion, which rules the friction-reduction properties of other materials such as 2D-layered materials, aromatic molecules, traditional S and P-based lubricant additives and MXenes with different terminations.

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QUANTIZED BORN EFFECTIVE CHARGES AS PROBES FOR THE TOPOLOGICAL PHASE TRANSITION IN THE HALDANE AND KANE-MELE MODELS

Paolo Fachin¹, Francesco Macheda¹, Paolo Barone² and Francesco Mauri¹

1 Dipartimento di Fisica, Universita' di Roma La Sapienza, Roma, Italy 2 CNR-SPIN, Area della Ricerca di Tor Vergata, Roma, Italy

A new approach to study the topological phase transitions, based on the assessment of the vibrational resonances in infrared spectra, is here proposed [1]. In the Haldane and Kane-Mele models the Born effective charges are nearly quantized, with a discontinuous jump associated with the topological phase transition, corresponding to a finite value in the trivial phase and a null one in the nontrivial one. This is explained by the connection between Born effective charges and electronic Berry curvature at the band edges [2]. Finally, at the topological phase transition of the Haldane model, due to the time-reversal symmetry breaking, a nearly quantized jump of the chiral splitting of the phonon frequencies is observed ([3][4][5]).

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MOLECULAR DYNAMICS SIMULATION OF ECO-FRIENDLY LUBRICANT ADDITIVES

Mauro Ferrario^{1,2}, Huong T. T. Ta², Alberto Pacini², Sophie Loehlé³ and M. C. Righi²

¹FIM Department, University of Modena and Reggio E., Modena, Italy ²Department of Physics and Astronomy, University of Bologna, Bologna, Italy ³TotalEnergies, OneTech Fuels&Lubricants, Research Center Solaize, Solaize, France.

With as much as 23% of the world's energy consumed in tribological contacts and the large majority of lubricants and additives still based on crude oil, the search for more environmentally friendly alternatives has become the priority to achieve substantial environmental impact in a sustainable manner. In particular the interest in aqueous-based lubricant has been amplified to fulfill the surging need for non-flammable, high specific heat capacity and high-performance lubricants for EV applications. The challenge is to simulate by molecular dynamics the relevant mechanochemistry and tribochemistry processes, that involve multiple physical/chemical interactions induced by extreme conditions including molecular confinement, high temperatures and mechanical stress applied. While force fields fall short reproducing the enhanced reactivity arising by quantum effects, ab initio molecular dynamics is severely limited by the complexity of the systems of interest, their sizes, and the long-time scale on which relevant events take place. To bridge the gap one needs to train robust and accurate inter-atomic potentials(IAP) based on machine-learning(ML) algorithms such as Deep-Neural Networks[1]. Here we shows successful applications of an active learning approach based onto Smart-Configuration-Sampling[2,3] developed specifically to construct tribochemistry-aware training datasets. Molecular Dynamics with tribologically-optimized ML-IAP models allowed us to unravel the mechanochemistry of formation and the friction reduction properties of carbon-based lubricious tribofilms, and confirm the great potential of pharmacopoeia-derived, naturally occuring, molecules such has hypericin and gallates when used as additives to obtain high performance lubricants for steel interfaces from water/glycerol/PAG solutions.

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These results are part of the "Advancing Solid Interface and Lubricants by First Principles Material Design (SLIDE)" project that has received funding from the European Research Council (ERC) under the European Union's Horizon 2020 research and innovation program (Grant agreement No. 865633).

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DESIGNING OPTIMAL CATALYST FOR HYDROGEN AND CARBON NANOTUBE PRODUCTION VIA METHANE PYROLYSIS

Vito Foderà & Maria Clelia Righi

Department of Physics and Astronomy "A. Righi", University of Bologna

Hydrogen production by methane pyrolysis, which occurs with the simultaneous capture of carbon in solid form, represents an appealing alternative to traditional H2 production methods as it avoids the recombination of C in CO2 [1]. In particular, the use of metallic nanoparticles as catalysts enables the growth of carbon nanotubes (CNTs). Despite extensive research on nickel, copper and other catalysts, the atomistic mechanisms of CH4 dissociation and CNTs growth on iron Fe and iron carbide Fe3C nanoparticles remain underexplored [2]. This study employs Density Functional Theory (DFT), and Machine Learning Force-Fields (MLFF) to investigate the initial stages of CH4 dissociation on Fe and Fe3C surfaces. We examined the physisorption, dissociative chemisorption and the energy barriers of CH4 dissociation on several Fe and Fe3C surfaces, chosen on the basis on the Wolff construction. The collected data were used to train a MLFF, enabling large-scale simulations over extended time periods. Both Fe3C and Fe demonstrated superior catalytic performance over traditional Ni- and Cu-based catalysts, iron carbide being the most reactive catalysts. Additionally, we evaluated the role of Cu, Mo, Mn, promoters in affecting methane dissociation and carbon diffusion. This study provides new insights into the catalytic mechanisms of ferrous materials, paving the way for improved catalytic processes for H2 production and environmental sustainability.

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PRESSURE INDUCED SUPERCONDUCTIVITY IN MERCURY SULFIDE

Pietro Maria Forcella [1], Cesare Tresca [2], Gianni Profeta [1,2]

Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy CNR-SPIN c/o Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy

Mercury chalcogenides are a class of materials that exhibit diverse structural phases under pressure, leading to a variety of intriguing and exotic physical properties such as topological phases, chiral phonons, etc. Following recent experiments^[1], in this work, we aim to study the pressure induced phase transition of mercury sulfide (HgS) and the rise of a superconducting phase when the crystal undergoes from the cinnabar phase (space group $P32_21$) to the rock salt phase (space group Fm-3m). Studying the phase diagram of HgS has consistently posed challenges, both experimentally and theoretically, with a wide range of uncertainty on the transition pressure. By means of Density Functional Theory (DFT) we investigated the phase transition of these two phases and the emergence of superconductivity, showing the critical features of such system.

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Session 2 – Thursday the 29th of August 2024 – 18:30-19:30

Matteo Furci	First-order rhombohedral to cubic phase transition in photoexcited GeTe
Federico Giannessi	The HEX database
Flavio Giuliani	Ab-initio study of supercooled antimony alloys through a machine learning interatomic potential
Mattia Iannetti	Edge states of the triangular QSH insulator indenene
Edoardo Marquis	DFT as a tool for designing low-friction materials
Francesca Martini	Optical properties of carbon nitrides for hydrogen production
Stefano Mocatti	Ultrafast dynamics of electrons and phonons: an ab initio computational perspective
Enrico Pedretti	XSORB: a software for identifying the most stable adsorption configuration and energy of a molecule on a crystal surface
Paolo Settembri	The spin density wave unfolded bands of Chromium
Cesare Tresca	Evidence of Molecular Hydrogen in the N-doped LuH3 System: a Possible Path to Superconductivity?
Stefano Paolo Villani	Ab-initio calculation of resonant Raman spectra of semiconductors
Giulio Volpato	Wannier interpolation of periodic and non-periodic operators in the optimally smooth subspace

FIRST-ORDER RHOMBOHEDRAL TO CUBIC PHASE TRANSITION IN PHOTOEXCITED GETE

Matteo Furci 1, Giovanni Marini 1,2, and Matteo Calandra 1,2,3

1 Department of Physics, University of Trento, Trento, Italy; 2 Graphene Labs, Fondazione Istituto Italiano di Tecnologia, Genova, Italy; 3 Sorbonne Université, CNRS, Institut des Nanosciences de Paris, Paris, France

Photoexcited GeTe undergoes a nonthermal phase transition from a rhombohedral to a rocksalt crystalline phase. The microscopic mechanism and the nature of the transition are unclear. By using constrained density functional perturbation theory and by accounting for quantum anharmonicity within the stochastic self-consistent harmonic approximation, we show that the nonthermal phase transition is strongly first order and does not involve phonon softening, at odds with the thermal one. The transition is driven by the closure of the single particle gap in the photoexcited rhombohedral phase. Finally, we show that ultrafast x-ray diffraction data are consistent with a coexistence of the two phases, as expected in a first order transition. Our results are relevant for the understanding of phase transitions and bonding in phase change materials.

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author(s) only and do not necessarily reflect those of the European Union or the European Research Council. Neither the European Union nor the granting authority can be held responsible for them.

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THE HEX DATABASE

Federico Giannessi, Simone Di Cataldo, Santanu Saha, Lilia Boeri

Università degli Studi Dell'Aquila

We introduce the HEX (High-pressure Elemental Xstal) database: a collection of the ground-state crystal structures of the first 57 elements of the periodic table (H-La) at 0, 100, 200 and 300 GPa. The scope of this work is to provide a unified reference for high-pressure research. It has been compiled by searching for all available experimental information on elements at high pressures, and complemented with accurate DFT-based simulations.

The HEX database provides both a reference for high-pressure physics, as well as a benchmark for *ab-initio* methods of crystal structure prediction: in 98% of the available cases, our simulations either coincide or are degenerate in enthalpy within 300 K with experimental crystal structure.

AB-INITIO STUDY OF SUPERCOOLED ANTIMONY ALLOYS THROUGH A MACHINE LEARNING INTERATOMIC POTENTIAL

Flavio Giuliani, Francesco Guidarelli Mattioli, John Russo, Lilia Boeri, Riccardo Mazzarello

Università di Roma 'La Sapienza', Italy

Antimony (Sb) and its alloys are a case study material, both for fundamental research on the structural glass transition and for applications as phase-change materials (PCMs).

Chalcogenide-based PCMs are at the core of innovative nanotechnology devices spanning from memory units to neuromorphic computing units. The phase-change behavior consists in a fast and reversible switching mechanism between a crystalline state and a glassy state, which are both stable at room temperature. The switching ability arises from the super-Arrhenius increase of viscosity during supercooling – this is known as fragile behavior, compared to the strong Arrhenius behavior. Explaining the behavior of a material's fragility at atomic level is therefore crucial, both for theoretical understanding of the glass transition and for PCM design and optimization. State-of-the-art theoretical studies of PCMs consist in training a machine-learned potential, usually a neural-network one (NNP), to predict the ground-state interatomic energies and forces computed via Density Functional Theory (or other ab initio methods); then using the NNP as a driver for more efficient but still ab initio molecular dynamics simulations on larger time- and space- scales. Efficient simulations allow an exhaustive sampling of the potential energy landscape (PEL) in

supercooled states; from the PEL data and through the Adam-Gibbs relation [1], one can compute the viscosity at low temperature, thus the material's fragility.

In this poster, we present preliminary results for the first ab initio computation of the fragility for bulk monoatomic Sb, using a NNP available from literature [2]. Sb is a candidate monoatomic PCM [3], whose glass lifetime can be engineered by nano-confinement or by chalcogenide doping. At atomic level, a competition between a regular and a Peierls-like distorted octahedral structure dictates the crystallization and amorphization of Sb-based PCMs. This suggests a possible fragile-to-strong transition (FST) arising from the competition of two structural environments during supercooling. Experimental hints of a FST are available for the germanium-doped alloy Ge15Sb85 [4]. Depending on the stage of our research, we may also show preliminary results for the training of new NNPs for Sb and Ge15Sb85.

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EDGE STATES OF THE TRIANGULAR QSH INSULATOR INDENENE

Mattia Iannetti¹, Jonas Erhardt^{2,3}, Cedric Schmitt^{2,3}, Simon Moser^{2,3}, Gianni Profeta^{1,5}, Domenico Di Sante⁴, Ralph Claessen^{2,3}, Giorgio Sangiovanni^{3,6}

¹Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy; ²Physikalisches Institut, Universität Würzburg, Würzburg, Germany; ³Würzburg-Dresden Cluster of Excellence ct.qmat, Universität Würzburg, Würzburg, Germany; ⁴Department of Physics and Astronomy, University of Bologna, Bologna, Italy; ⁵CNR-SPIN C/o Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy; ⁶Institut für Theoretische Physik und Astrophysik, Universität Würzburg, Würzburg, Germany

Quantum Spin Hall Insulators (QSHI) are promising materials for many applications based on Dirac fermions and topologically-protected edge states. Indium adatoms on a silicon carbide surface, the so-called Indenene, was the the first material in which a topological classification solely based on an inspection of the bulk wave functions has been demonstrated [1]. Moreover, its graphene capping offers an ambient condition stability that is crucial for future utilization [2]. However, the experimental observation of Indenene edge-states is still lacking. In this poster, we present a theoretical analysis of finite-sized Indenene systems using a quantitative tight binding model on different geometric configurations, highlighting the reach physics of edge-states and their interaction, in support of their experimental measurements.

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DFT AS A TOOL FOR DESIGNING LOW-FRICTION MATERIALS

Edoardo Marquis

Department of Physics and Astronomy, University of Bologna

Friction and wear are common phenomena, causing massive economic and environmental costs. Reducing friction could save substantial amounts of energy and material losses, highlighting the need for effective low-friction materials.^[1] Density Functional Theory (DFT) simulations play a crucial role in this effort by aiding both experimental design and fundamental understanding. Indeed, DFT can help in screening potential lubricating materials, reducing the necessity for numerous and expensive laboratory experiments. Also, simulations can provide insights into the mechanisms at the interfaces of micro- and nano-asperities in contact, which are difficult to observe in real experiments. Within this context, I will present some case studies concerning the *ab initio* study of two-dimensional (2D) layered materials. These materials, composed by thin layers interacting through weak Van der Waals forces, very often allow easy shear and low friction. Among the most recent and rich families of 2D layered materials, MXenes,^[2] Transition Metal Dichalcogenides (TMDs)^[3] and Transition Metal Carbo-Chalcogenides (TMCCs)^[4] offer promising lubricating properties. By simulating how these materials respond to shear and external loads, DFT provides insights into their potential as solid lubricants.



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OPTICAL PROPERTIES OF GRAPHITIC CARBON NITRIDES FOR WATER SPLITTING

Francesca Martini

Department of Physics, University of Trento, Povo, Italy

Over the past several years, the search for sustainable and clean energy sources has gained unprecedented importance in addressing the challenges posed by climate change; hydrogen is the chemical fuel with the highest energy density of 140 MJ/Kg but a photocatalyst with a reasonable band gap is needed for the process.

Lately, graphitic C₃N₄ (g-C₃N₄) has attracted much attention for its high thermal and chemical stability and non-metallicity. In literature, two building blocks of g-C₃N₄ are considered: s-triazine and tri-s-triazine (or heptazine), which is known to be more stable than the other polytype [1]. Furthermore, it is now known that these structures present some level of corrugation. Re Fiorentin et al. [2] studied how the corrugation of these structures alters the electronic and optical properties of the two polytypes, calculating the absorption spectrum in the GW+BSE scheme.

Starting from this article, the loss function at different transferred momentum was calculated, obtaining the excitonic band structure for both polytypes. The calculations show that excitons in these materials present the typical linear dispersion of Frenkel exciton in 2D materials. Furthermore, low-energy excitons in tri-s-triazine g-C₃N₄ are found to be strongly localized and with negligible dispersion.



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ULTRAFAST DYNAMICS OF ELECTRONS AND PHONONS: AN AB INITIO COMPUTATIONAL PERSPECTIVE

Stefano Mocatti, Giovanni Marini, Pierluigi Cudazzo, Matteo Calandra

Department of Physics, University of Trento, Povo, Italy

The computational modeling of photoexcited semiconductors is a powerful tool for understanding the physical mechanisms underlying light-driven phenomena. Recent real-time simulations have demonstrated significant predictive power and provided rich physical insights [1-2], highlighting the potential for exploiting photoexcited materials in technological applications. However, the complex interplay of light-matter, electron-electron, electron-phonon, and phonon-phonon interactions poses significant challenges in predicting the realistic behavior of materials following photoexcitation, primarily due to the high computational cost.

Here, we present an ab initio computational scheme within the EPIq code [3], which combines the semiconductor Bloch equations with semiclassical Boltzmann dynamics, treating all interactions on an equal footing. This workflow enables the real-time evolution of electron and phonon occupations, polarization, and nuclear motion at a manageable computational cost. We showcase the capabilities and predictive power of this scheme using monolayer hBN and MoS2 as case studies. The results reveal a clear separation of the timescales associated with each interaction and their significance in the relaxation towards quasi-equilibrium. This work bridges the gap between out-of-equilibrium and quasi-equilibrium states, advancing the understanding of nonequilibrium light-driven phenomena on short timescales.

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XSORB: A SOFTWARE FOR IDENTIFYING THE MOST STABLE ADSORPTION CONFIGURATION AND ENERGY OF A MOLECULE ON A CRYSTAL SURFACE

E. Pedretti, P. Restuccia, M. C. Righi

Dipartimento di Fisica e Astronomia, Università di Bologna, Bologna (Italy)

Molecular adsorption is the first important step of many surface-mediated chemical processes, from catalysis to lubrication. This phenomenon is controlled by physical/chemical interactions, which can be accurately described by first-principles calculations. Several computational tools have been developed to study molecular adsorption based on high throughput/automatized approaches in recent years. However, these tools can sometimes be over-sophisticated for non-expert users. Here we present Xsorb, a Python-based program for identifying the accurate adsorption energy and geometry of complex molecules on crystalline (reconstructed) surfaces. The program automatically samples the potential energy surface (PES) that describes the molecule-surface interaction by generating several adsorption configurations through symmetry operations. The set of the most representative ones is automatically identified through a fast pre-optimization scheme. Finally, the PES global minimum is identified through a full structural optimization process. We show the program capabilities through an example consisting of a hydrocarbon molecule, 1hexene, adsorbed over the (110) surface of iron and the reconstructed (001) surface of diamond. This program, despite its conceptual simplicity, is very effective in reducing the computational workload usually associated with the creation and optimization of several adsorption configurations.



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THE SPIN DENSITY WAVE UNFOLDED BANDS OF CHROMIUM

F. Bisti [1,2], **P. Settembri** [1], J. Minár [3], V. A. Rogalev [2], R. Widmer [4], O. Gröning [4], M. Shi [2], T. Schmitt [2], G. Profeta [1,5], and V. N. Strocov [2]

[1] Dipartimento di Scienze Fisiche e Chimiche, Università dell'Aquila, L'Aquila, Italy;
 [2] Swiss Light Source, Paul Scherrer Institute, Villigen PSI, Switzerland;
 [3] New Technologies Research Center, University of West Bohemia, Pilsen, Czech Republic;
 [4] nanotech@surfaces Laboratory, EMPA, Swiss Federal Laboratories for Materials Science and Technology, Duebendorf, Switzerland;
 [5] CNR-SPIN L'Aquila, L'Aquila, Italy

Chromium represents the classic example of traveling antiferromagnet: its incommensurate spin density wave (SDW) has a wave vector Q determined by the nesting properties of its Fermi surface. Surprisingly, such extremely simple metal has not found a satisfactory reconciliation between experimental magnetic order and electronic bands structure within the density functional theory framework. We report its electronic structure investigation by soft-X-ray angle resolved photoemission spectroscopy thus providing a bulk oriented exploration. The Fermi surface contours along the plane parallel to the (100) crystal surface precisely match the nesting conditions, highlighting also signal coming from the magnetic order. The probed band dispersion found an excellent explanation once the spin density wave is stabilized within density functional theory and the calculated states are weighted with the projections on the body-centered cubic crystal. Finally, with one-step photoemission calculations we demonstrate the role of final states in the formation of a multitude of replica bands in the ARPES signal. Surprisingly, the free-electron model final state results to be a bad approximation for the investigated crystal surface even at excitation photon energy up to 1 keV.



EVIDENCE OF MOLECULAR HYDROGEN IN THE N-DOPED LUH₃ SYSTEM: A POSSIBLE PATH TO SUPERCONDUCTIVITY?

Cesare Tresca¹, Pietro Maria Forcella², Andrea Angeletti^{3,4}, Luigi Ranalli^{3,4}, Cesare Franchini^{4,5} Michele Reticcioli⁴ and Gianni Profeta^{2,1}

¹ CNR-SPIN c/o Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy; ² Dipartimento di Scienze Fisiche e Chimiche, Università degli Studi dell'Aquila, L'Aquila, Italy; ³ University of Vienna, Vienna Doctoral School in Physics, Vienna, Austria; ⁴

University of Vienna, Faculty of Physics and Center for Computational Materials Science, Vienna, Austria; ⁵ Dipartimento di Fisica e Astronomia, Università di Bologna, Bologna, Italy

The discovery of ambient superconductivity would mark an epochal breakthrough long-awaited for over a century, potentially ushering in unprecedented scientific and technological advancements. The recent findings on high-temperature superconducting phases in various hydrides under high pressure have ignited optimism, suggesting that the realization of near-ambient superconductivity might be on the horizon. However, the preparation of hydride samples tends to promote the emergence of various metastable phases, marked by a low level of experimental reproducibility. Identifying these phases through theoretical and computational methods entails formidable challenges, often resulting in controversial outcomes. In this paper, we consider N-doped LuH₃ as a prototypical complex hydride: By means of machine-learning-accelerated force-field molecular dynamics, we have identified the formation of H₂ molecules stabilized at ambient pressure by nitrogen impurities. Importantly, we demonstrate that this molecular phase plays a pivotal role in the emergence of a dynamically stable, low-temperature, experimental-ambient-pressure superconductivity. The potential to stabilize hydrogen in molecular form through chemical doping opens up a novel avenue for investigating disordered phases in hydrides and their transport properties under near-ambient conditions.

AB-INITIO CALCULATION OF RESONANT RAMAN SPECTRA OF SEMICONDUCTORS

Stefano Paolo Villani^(a), Paolo Barone^(b), Francesco Mauri^(a)

(a) Sapienza Università di Roma, (b) CNR-SPIN

Since its first realization, vibrational Raman spectroscopy has become one of the most widely used optical techniques in materials science. It allows for the determination of structural properties and new phases even at extreme conditions, where other techniques fail or are less readily available and it can be also used in the absence of long-range structural order as for liquid or amorphous materials. First-principles calculation of Raman spectra is thus highly desirable, allowing to associate Raman lines to specific microscopic structures. Within density functional theory, the standard approach for the calculation of vibrational Raman intensities in periodic systems, relies on second order derivatives of the electronic densities with respect to a static uniform electric field[1,2]. The advantage with respect to other approaches relies in the negligible computational effort required for the evaluation of the intensities, compared to that required for the calculation of vibrational frequencies, allowing for the determination of Raman spectra in large systems up to several hundreds of atoms. However, this technique is limited to the treatment of static electric fields, failing to account for (near-)resonant effects present in semiconductors. In this work, we propose a generalization of the second-order approach for the treatment of non-static electric fields, which keeps the computational advantage and thus allows for the efficient calculation of resonant Raman spectra in large semiconductors.

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WANNIER INTERPOLATION OF PERIODIC AND NON-PERIODIC OPERATORS IN THE OPTIMALLY SMOOTH SUBSPACE

Giulio Volpato, Giovanni Marini, Matteo Calandra

Department of Physics, University of Trento, Trento, Italy

Linear response calculations of the electron-phonon coupling have a substantial computational cost since an independent calculation is required at each phonon momentum. However, dense electron and phonon momentum grids are required in order to achieve convergence, hence, an interpolation scheme is required. A popular one is based on the Wannier interpolation¹⁻⁴. In this scheme, the deformation potential is calculated in the maximally localized Wannier function basis and then Fourier interpolated.

Here, within the Wannier interpolation approach, we develop a new interpolation scheme, which takes full advantage of the optimally smooth subspace defined by the MLWF's to perform a direct interpolation in reciprocal space. We compare the two methods for the case of MgB₂ and single layer MoS_2 with an ab-initio calculation. Results show that this new scheme yields more accurate results at a comparable computational cost compared to the existing method. Moreover, it also allows for the interpolation of lattice non-periodic objects, such as the oscillator strength in the phonon momentum, which is not available with the Fourier scheme.

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