CMT@BRIXEN

5th-7th June 2023

The Meeting of the
Condensed Matter Theory Italian Community

PROGRAM & BOOK OF

ABSTRACTS

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Program

Monday the 5th of June 2023

From 8.00 onwards Registration

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11:40-12:15 Invited: **Francesco Scazza –** ***Probing correlated fermionic Systems with single-Quantum Control***
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Tuesday the 6th of June 2023

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TALKS

Monday 5th of June 2023

Quantum Science and Technologies (9:00-12:50)

9:00-10:00 (Keynote)

EXPLORING THE ENTANGLEMENT STRUCTURE OF MANY-BODY WAVEFUNCTIONS ON A QUANTUM SIMULATOR

Peter Zoller

Institute for Theoretical Physics, University of Innsbruck, and IQOQI, Austrian Academy of Sciences, Austria

Uncovering the entanglement structure of many-particle wavefunctions in quantum simulation experiments is a fundamental challenge in quantum information science. In a theory-experiment collaboration, we have prepared ground and excited states of a 1D XXZ Heisenberg chain using variational algorithms on a 51-ion programmable quantum simulator, and we have utilized sample-efficient tomography to "learn" the operator structure of the Entanglement Hamiltonian for subsystems up to 20 lattice sites. We provide clear evidence for a local structure of the Entanglement Hamiltonian, implying that the reduced state takes the form of a Gibbs ensemble, with a spatially-varying temperature profile as a signature of entanglement. For ground states our findings are in quantitative agreement with predictions of Bisognano and Wichmann adapted to lattice models. Our results also show the transition from area to volume-law scaling of Von Neumann entanglement entropies from ground to excited states. We anticipate that our findings and methods have wide-ranging applicability to revealing and understanding entanglement in many-body problems with local interactions including higher spatial dimensions.

Monday 5th of June 2023

Quantum Science and Technologies (9:00-12:50)

10:00-10:35

DEEP LEARNING THE FUNCTIONAL RENORMALIZATION GROUP FLOW FOR CORRELATED FERMIONS

Domenico Di Sante

University of Bologna, Italy

I will present a data-driven dimensionality reduction of the scale-dependent 4-point vertex function characterizing the functional Renormalization Group (fRG) flow for the widely studied two-dimensional t − t' Hubbard model on the square lattice. It will be shown that a deep learning architecture based on a Neural Ordinary Differential Equation solver in a low-dimensional latent space efficiently learns the fRG dynamics that delineates the various magnetic and d-wave superconducting regimes of the Hubbard model. In addition, a Dynamic Mode Decomposition analysis confirms that a small number of modes are indeed sufficient to capture the fRG dynamics. This talk will demonstrate the possibility of using artificial intelligence to extract compact representations of the 4-point vertex functions for correlated electrons, a goal of utmost importance for the success of cutting-edge quantum field theoretical methods for tackling the many-electron problem. Besides the specific application to correlated fermions, I will discuss a dimensionality reduction scheme that may be useful to any research field dealing with presumable very high-dimensional data.

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Monday 5th of June 2023

Quantum Science and Technologies (9:00-12:50)

11:05-11:40

(2+1)D SU(2) YANG-MILLS LATTICE GAUGE THEORY AT FINITE DENSITY VIA TENSOR NETWORKS

Pietro Silvi

University of Padova, Italy

We demonstrate the feasibility of Tensor Network simulations of non-Abelian lattice gauge theories in two spatial dimensions. In particular, we focus on a SU(2) Yang-Mills model in the Hamiltonian formulation, including dynamical matter. Our sign-problem-free approach allows for characterizing the phase diagram of the model at zero and finite charge densities, as a function of the bare mass and the coupling constant g. We observe a transition, driven by g, from a phase with dominant electric fluctuations to a phase with dominant magnetic fluctuations. For the smallest nontrivial representation of the gauge field, at low values of the bare mass the deconfined regime is replaced by a superconducting phase of colorless mesons. In this representation, our simulations suggest that topological order does not survive within this phase, but it still may appear at the critical point.

Monday 5th of June 2023

Quantum Science and Technologies (9:00-12:50)

11:40-12:15

PROBING CORRELATED FERMIONIC SYSTEMS WITH SINGLE-QUANTUM CONTROL

Francesco Scazza

University of Trieste and CNR-INO, Italy

Ultracold atoms provide an exciting playground for exploring quantum many-body phenomena, owing to an exceptional control over the Hamiltonians and their long coherent time scales. Exciting developments have recently extended the experimental capabilities down to the single-quantum control and detection. In particular, high-resolution optical traps allow for microscopically controlling atomic many-particle systems, or even assembling defect-free arrays of hundreds of atoms. In this talk, I will first focus on recent experiments where we have precisely engineered few- and many-vortex states in fermionic superfluids, exploring their dynamics by single-quantum vortex tracking. I will then report on the ongoing efforts to construct a new experimental apparatus in Trieste, aiming to trap, control and detect individual two-electron atoms. This will allow us to study mesoscopic fermionic many-body systems from a bottom-up perspective, assisted by the precise atomic clock toolbox of two-electron atoms, exploring a wide range of strong correlation phenomena in itinerant Fermi systems.

Monday 5th of June 2023

Quantum Science and Technologies (9:00-12:50)

12:15-12:50

QUANTIFYING NON-STABILIZERNESS IN MANY-BODY SYSTEMS

Emanuele Tirrito

SISSA, Trieste, Italy

Non-stabilizerness – also colloquially referred to as magic – is a resource for advantage in quantum computing and lies in the access to non-Clifford operations. Developing a comprehensive understanding of how non-stabilizerness can be quantified and how it relates other quantum resources is crucial for studying and characterizing the origin of quantum complexity. In this presentation, I will establish a direct link between non-stabilizerness and entanglement spectrum flatness for a pure quantum state. This connection can be exploited to efficiently investigate non-stabilizerness, even in the presence of noise. Furthermore, I will illustrate a Monte Carlo approach applied to probability distribution of Pauli strings to estimate non-stabilizerness, which is quantified by the Stabilizer Renyi Entropies (SREs). This will provide an insightful and efficient method for characterizing and analyzing the role of non-stabilizerness in quantum many-body systems.

Monday 5th of June 2023

Electronic Excitations and ultrafast Spectroscopy (14:30-18:20)

14:30-15:30 – Keynote

THE MODELING OF LIGHT-INDUCED PROCESSES IN MOLECULES EMBEDDED IN COMPLEX ENVIRONMENTS

Benedetta Mennucci

Department of Chemistry, University of Pisa, Italy

The response to light of molecules can significantly change when they are embedded in complex environments. The modeling of these specific responses can only be revealed by computational approaches which are able to couple structural, electronic and dynamic properties of the molecules and the embedding system. A possible strategy is to couple quantum chemistry and classical models and integrate the resulting multiscale approach into dynamics, but many theoretical and numerical critical issues have to be faced. In this talk, these issues will be discussed, and possible solutions will be presented together with some applications.

Monday 5th of June 2023

Electronic Excitations and ultrafast Spectroscopy (14:30-18:20)

15:30-16:05

ABINITIO APPROACH TO MODEL EXCITONS IN PUMP AND PROBE EXPERIMENTS

Davide Sangalli

Istituto di Struttura della Materia-CNR (ISM-CNR). Monterotondo, Italy

In this talk I present a first principles approach to model pump and probe experiments. Starting from a general discussion on carriers generation, I focus on the description of non-equilibrium excitonic states with ultra-short laser pulses. The modelling is achieved via the real-time propagation of the density matrix, within the time-dependent Hartree plus Screened EXchange (TD-HSEX) approaximation. The generated density matrix can be used to model transient spectroscopy signals in the presence of strongly bound excitons. Using LiF as a prototype material, I show that the scheme is able to capture the exciton signature both in time-resolved angle-resolved photoemission spectroscopy and transient absorption experiments [1-3]. The approach is general and can become the reference scheme for modeling pump and probe experiment in a wide range of materials. In the last part of the talk. I'll discuss the coupling of excitons with phonons and the the calculation of exciton-phonon lifetimes [4-5].

ACKNOWLEDGMENTS
The results presented in this talk are part of collaborations with C. Attaccalite, A. Marini, E. Perfetto, and G. Stefanucci.
The developments are freely available in the Yambo code (www.yambo-code.eu).
I also aknowledge financial support from:
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Monday 5th of June 2023

Electronic Excitations and ultrafast Spectroscopy (14:30-18:20)

16:35-17:10

LIGHT-TUNABLE ULTRAFAST PHENOMENA IN QUANTUM MATERIALS

Giovanni Marini

Istituto Italiano di Tecnologia, Italy

The use of ultrashort coherent light pulses to design and manipulate materials is a hot topic in condensed matter physics because it allows for control over a wide range of material properties as well as the observation of hidden broken-symmetry states. I talk about the role of first principles techniques in understanding ultrafast physical phenomena, with a particular emphasis on the inherent theoretical difficulties associated with the description of out-of-equilibrium systems. Finally, I discuss a novel approach to modeling insulators exposed to ultrafast pulses [1,2] as well as some real-world applications.

ACKNOWLEDGMENTS
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Monday 5th of June 2023

Electronic Excitations and ultrafast Spectroscopy (14:30-18:20)

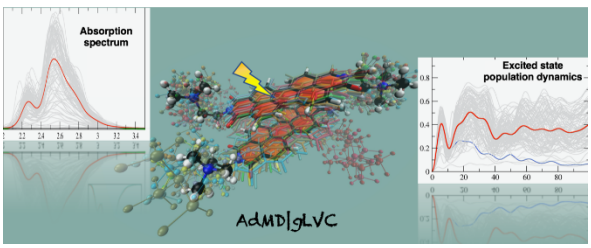
17:10-17:45

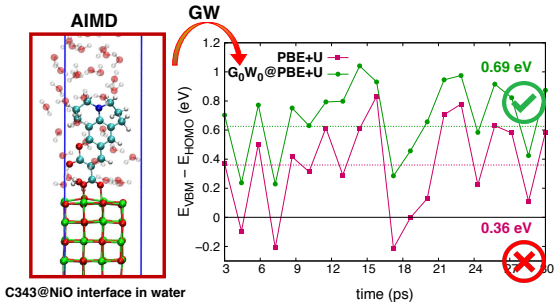
MULTISCALE MODELING OF PHOTOACTIVE MATERIALS AND INTERFACES FOR SOLAR ENERGY CONVERSION

Mariachiara Pastore

Université de Lorraine & CNRS, Laboratoire de Physique et Chimie Théoriques (LPCT), Nancy, France

In the context of solar energy exploitation, dye-sensitized solar cells (DSCs) and dye-sensitized photoelectrosynthetic cells (DSPECs) offer the promise of cost-effective sunlight conversion and storage, respectively. Dye-functionalization of bot n- and p-type semiconductors (like TiO_2 and NiO) can be either exploited to build active DS photoelectrodes or tandem DSC and DSPECs devices. Computational modelling has played a prominent role in the development of the DSC technology, affording accurate prediction of both isolate components (dye's optical properties, catalysts, and redox mediators, etc…) and semiconductor sensitization (structure, electronic structure, optical properties, charge transfer kinetics). Here I will discuss the recent advances concerning first principles modeling of materials, interfaces, and processes of n- and p-type photoelectrodes. In the first part of the talk, I will present the recent development of hybrid classical/QM approaches for the simulation of steady-state and transient absorption and emission spectra of molecular dyes and their aggregates in solution [1,2,3]. Then, moving sensitized semiconductor interfaces, I will discuss the modeling of electronic and structural properties of the complex NiO/solvent/dye interface, whose characterization is still poor when compared to the level of understanding reached for TiO_2 sensitized photoanodes, from both the experimental and computational point of view.[4] I will address the problem of accurately predicting the energy level alignment across the dye/semiconductor interface by state of the art DFT and large scale GW calculations and the challenging definition of a proper structural model needed to reliably capture the interface complexity.





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Monday 5th of June 2023

Electronic Excitations and ultrafast Spectroscopy (14:30-18:20)

17:45-18:20

ATTOSECOND MAGNETIZATION DYNAMICS DRIVEN BY INTENSE FEMTOSECOND LASERS

Nicolas Tancogne-Dejean

Max Planck Institute for Structure and Dynamics of Matter, Hamburg, Germany and European Theoretical Spectroscopy Facility (ETSF)

Irradiating solids with ultrashort laser pulses is known to initiate femtosecond timescale magnetization dynamics [1]. However, subfemtosecond spin dynamics have not yet been observed or predicted. Here, we explore ultrafast light-driven spin dynamics in a highly nonresonant strong-field regime [2]. Through state-of-the-art ab initio calculations, we predict that a nonmagnetic material can transiently transform into a magnetic one via dynamical extremely nonlinear spin-flipping processes, which occur on attosecond timescales and are mediated by cascaded multi-photon and spin–orbit interactions. These are nonperturbative nonresonant analogs to the inverse Faraday effect, allowing the magnetization to evolve in very high harmonics of the laser frequency (e.g. here up to the 42nd, oscillating at ~100 attoseconds), and providing control over the speed of magnetization by tuning the laser power and wavelength. Remarkably, we show that even for linearly polarized driving, where one does not intuitively expect the onset of an induced magnetization, the magnetization transiently oscillates as the system interacts with light. This response is enabled by transverse light-driven currents in the solid, and typically occurs on timescales of ~500 attoseconds (with the slower femtosecond response suppressed). An experimental setup capable of measuring these dynamics through pump–probe transient absorption spectroscopy is simulated. Our results pave the way for attosecond regimes of manipulation of magnetism.

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Tuesday 6th of June 2023

Materials Theory (9:00-12:50)

9:00-10:00 – Keynote

METAL-HALIDE PEROVSKITES: A WONDER SEMICONDUCTOR CLASS FOR SOLAR CELLS AND OPTOELECTRONIC APPLICATIONS

Filippo de Angelis

Dipartimento di Chimica, Biologia e Biotecnologie, Università degli Studi di Perugia and INSTM, and Computational Laboratory for Hybrid/Organic Photovoltaics (CLHYO), CNR-ISTM and University of Perugia, Perugia, Italy.

Metal-halide perovskites (MHPs) have been long-time known, but the interest in this class of compounds was revitalized in 2012 by the first breakthrough reports of efficient solid-state solar cells. An unprecedented "gold rush" led to currently certified >25% efficient single-junction solar cells, bringing the technology to rival with established PV technologies. Key to such efficiency records are the perovskite tuneable bandgap and the long lifetime of photogenerated charge carriers, whose origin is still debated. The latter property is likely due to a combination of defect tolerance, relativistic band structure and unusual electron-phonon coupling. In addition ionic and spin-orbital degrees of freedom can be manipulated by material and structure selection. These characteristics can be exploited in a variety of innovative devices, beyond solar cells. The high-performance compositions for solar cells, mainly relying on Pb-based compounds, but there is huge scope for device-oriented material design for new technology with tailored opto-electro-ion-spin-tronic properties. These include multifunctional energy conversion technologies and electronic devices exploiting ion and spin channels. Theoretical and computational modeling are complementary tools for rationalizing experimental results, on the one hand, and to direct experiments and device fabrication towards innovative concepts, on the other hand. These combined ingredients constitute the basis for development of new materials with similar target characteristics, possibly avoiding the environmental risks posed by lead, and opening the way towards tailored device-oriented materials selection with a range of unique properties to support to future technology breakthroughs.

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Tuesday 6th of June 2023

Materials Theory (9:00-12:50)

10:00-10:35

Flexoelectricity and long-Range Coulomb Interactions in two-dimensional Crystals

Massimiliano Stengel

ICREA, Barcelona, Spain

Curvature is ubiquitous at the nanoscale, either in the form of ripples or thermal excitations. It can have a dramatic impact on the physical properties of two-dimensional (2D) crystals or membranes, leading to exciting new functionalities of current technological interest. A notable example is flexoelectricity, whereby a flexural deformation induces an electrical response, either in the form of an open-circuit voltage or a polarization. A microscopic theory of the effect has been elusive until very recently, due to the lack of adequate computational methodologies to treat curvature in a density-functional context. In this talk I will outline the technical advances, within the framework of first-principles electronic-structure theory, that allowed us to lift this limitation. These revolve around two key fundamental achievements: (i) the ability to describe spatial dispersion effects (i.e., the response to modulated fields in the long-wavelength limit) perturbatively, and (ii) the correct treatment of long-range Coulomb interactions up to an arbitrary multipolar order. To illustrate the recently developed methodologies and the new opportunities they offer, I will present applications to a variety layered 2D crystals, emphasizing the connection to the existing models and the practical implications of our results.

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Tuesday 6th of June 2023

Materials Theory (9:00-12:50)

11:05-11:40

PREDICTING THE ELECTRONIC FREE ENERGY AT FINITE TEMPERATURE FROM GROUND STATE DATA

Federico Grasselli

EPFL, Lausanne, Switzerland

Machine-learning (ML) interatomic potentials, while extremely successful in describing condensed phases, are usually trained on ground-state electronic-structure calculations depending exclusively on the atomic positions and ignoring the electronic temperature. Hence, they are limited in their ability to describe thermally excited electrons. We introduce a rigorous ML framework to predict the finite-temperature electron free energy that is based exclusively on ground-state total energy and electronic density of states [1]. Our physically-motivated ML approach makes it possible to sample on-the-fly the electronic free energy at any temperature, and facilitates modeling material properties in extreme conditions with a fraction of the usual cost. We demonstrate it by computing the equation of state and heat capacity of metallic hydrogen at planetary conditions. This approach demonstrates the impact of a universal model describing structural and electronic properties inexpensively and its ability to enable more accurate and predictive materials modeling and design.

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Tuesday 6th of June 2023

Materials Theory (9:00-12:50)

11:40-12:15

TOWARDS HIGH-MOBILITY 2D SEMICONDUCTORS THROUGH ACCURATE AND AUTOMATED SIMULATIONS

Marco Gibertini

University of Modena, Italy

Charge transport plays a crucial role in manifold potential applications of two-dimensional materials and at most operating temperatures it is hindered by scattering of carriers by lattice vibrations. Assessing the intrinsic phonon-limited carrier mobility is thus of paramount importance to identify or engineer promising candidates for next-generation devices. Here, on one side, we provide a robust workflow to compute electron-phonon interactions and solve the corresponding Boltzmann equation towards an automated calculation of mobility in 2D semiconductors [1], including the effect of nearby layers forming a van der Waals heterostructure. Not only we profile best conducting materials [2] from a recent portfolio of 2D semiconductors [3], but we also illustrate strategies to boost the mobility of otherwise "poor" materials [4,5], with emphasis on the introduction of a metallic layer in the heterostructure whose free carrier screening remotely suppresses electron-phonon interactions in the current-carrying layer [5]. We use GaSe as a prototype, and place it in an heterostructure with doped graphene as the "screener" layer and BN as a separator. Remote screening leads to an enhancement by a factor 3 in GaSe, with a mobility that is almost constant, around 500 to 600 cm^2/Vs, over a wide range of carrier densities from 10^{11} to 10^{13} cm^{-2}pastore. On another side, we also discuss how to improve the efficiency of electron-phonon calculations through Fourier-Wannier interpolation by extending a recent formulation of long-range contributions to dynamical matrices and phonon dispersions in 2D [6], including the effect of dynamical dipoles and quadrupoles. Remarkably, we identify an unprecedented contribution associated with the Berry connection that is crucial to preserve the Wannier-gauge covariance of the theory [7]. We show the importance of the current strategy to fully account for the peculiar nature of long-range electrostatics in two dimensions by studying a wide selection of relevant monolayers [8].

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Tuesday 6th of June 2023

Materials Theory (9:00-12:50)

12:15-12:50

NON-COVALENT VAN DER WAALS INTERACTIONS: A LONG-RANGED COUPLING BETWEEN ELECTRONIC MODES AND IONIC LATTICE

Alberto Ambrosetti

University of Padova, Italy

Non-covalent van der Waals (vdW) interactions are extremely long-ranged, and crucially influence structural, dynamical and response properties of nanostructures and biomolecules. Many of the biological processes that enable life, countless interface phenomena, or even the assembly of nanomaterials deeply rely on vdW interactions. These forces have a truly quantum mechanical nature, and exhibit strong many-body effects. By introducing a reliable quantum many-body mechanical approach for dispersion interactions - which is equivalent to therandom phase approximation in the long-range limit -, here show that:
i) many-body correlations can make vdW interactions even longer-ranged than expected in nanoscale systems
ii) due to the interplay with many-body correlations, a strong coupling can arise between geometry and vdW interactions at he nanoscale
ii) many-body vdW interactions can amplify the sensitivity of nanostructures to mechanical stress
iii) optical excitations can induce highly non-local deformations, implying a coupling to collective phonon modes

Tuesday 6th of June 2023

Quantum Many-Body Systems: Materials and Methods (14:30-17:45)

14:30-15:30 – Keynote

A novel platform for topological superconductivity in multiband and multiorbital systems

Roberta Citro

Dipartimento di Fisica "*E.R. Caianiello*" & CNR Spin, Università degli Studi di Salerno, Italy

I will first review the properties of toy-models for topological superconductivity, the Kitaev chain and its generalizations. After discussing the topological phase diagram of the isolated system, using a scattering technique within the Bogoliubov–de Gennes formulation, I will discuss the differential conductance properties as a function of all relevant model parameters [1]. The relevant problem of implementing local spectroscopic measurements to characterize the Majorana fermions useful in quantum technologies is also addressed. Then, I will present a novel platform for topological superconductivity based on 2DEGs at LAO/STO interface. Here the interplay of spin-orbit interaction and intrinsic superconductivity may induce a topological phase transition in an applied magnetic field with strong orbital character [2,3]. The conclusions will address the design of various nanowire-based mesoscopic devices for topological computation [4,5].

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Tuesday 6th of June 2023

Quantum Many-Body Systems: Materials and Methods (14:30-17:45)

15:30-16:05

SOLVING QUANTUM IMPURITY PROBLEMS WITH MATRIX-PRODUCT STATES IN THE TEMPORAL DOMAIN

Alessio Lerose

University of Geneva, Switzerland

We introduce an efficient method to simulate dynamics of an interacting quantum impurity coupled to non-interacting fermionic reservoirs, based on a matrix-product state (MPS) encoding of the reservoir's Feynman-Vernon influence functional (IF). The efficiency of such representation rests on the moderate entanglement of the IF "temporal wavefunction" - dubbed temporal entanglement (TE). By analytically studying TE for the class of reservoirs relevant to quantum impurity problems, we establish that TE scales at most logarithmically with time. This provides theoretical guarantees of polynomial complexity of our method. We describe an explicit algorithm to encode a Gaussian IF into a MPS. We apply our method to quantum quenches and non-equilibrium transport in the strongly correlated regime of the Anderson impurity model, and find favorable performance compared to state-of-the-art methods.

Tuesday 6th of June 2023

Quantum Many-Body Systems: Materials and Methods (14:30-17:45)

16:35-17:10

HIDDEN QUANTUM STATES WITH BROKEN TIME REVERSAL SYMMETRY IN STRONGLY CORRELATED ELECTRON-PHOTON SYSTEMS

Giacomo Mazza

University of Pisa, Italy

Spontaneous symmetry breaking can triggers coupling between order parameters of the same symmetry. In this talk, I will discuss phase transitions of coupled electronic and photonic degrees of freedom leading to time-reversal symmetry broken (TRSB) states of purely orbital origin. The phase transition is driven by strong electronic correlations which trigger the breaking of lattice symmetries. The emergent TRSB state is controlled by engineered geometrical constraints which enable the coupling between correlated electrons and transverse degrees of freedom of the free space electromagnetic field. I will discuss implication for the control of electron-lattice coupled phase transition.

Tuesday 6th of June 2023

Quantum Many-Body Systems: Materials and Methods (14:30-17:45)

17:10-17:45

NEMATICITY IN STRONGLY CORRELATED SYSTEMS

Laura Fanfarillo

CNR-ISC, Italy

Electronic nematic phases are ordered states where electrons spontaneously break the rotational point-group symmetry of the crystal, but not its translational symmetry. In several quantum materials characterized by strong electronic correlations, including copper- and iron-based superconductors, a large anisotropy in the electronic properties, has been identified as a signature of electronic nematic order. Regardless of the origin of the nematic instability, the characterization of the nematic phase as emerging from experiments clearly calls for a theoretical scheme which includes the sizable electron-electron interactions and the consequent correlation effects of those systems. In this talk I will discuss the physics emerging from the interplay of electronic correlations and nematicity. I will highlight the differences occurring in Mott-like systems, in which correlations effects are ultimately controlled by a strong density-density on-site repulsion, and in Hund's metals, in which correlations are influenced by a large value of the exchange Hund's coupling. I will clarify how the nematic order is affected by the large effective mass renormalizations of the correlated system [1], as well as the relevance of the inclusion of the dynamical properties of the correlated system itself to understand the different interplay of nematicity and correlations at different energy scales [2]. I will finally connect our theoretical results with recent experimental findings in iron-based materials.

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Wednesday 7th of June 2023

Superconductivity and Topology (9:00-12:50)

09:00-10:00 – Keynote

TOPOLOGICAL SUPERCONDUCTIVITY: PERSPECTIVES AND PROSPECTS

Ronny Thomale

Julius-Maximilians-Universität Würzburg, Austria

Topological aspects of superconductivity have become a ubiquitous area of research in contemporary condensed physics. I will provide a synopsis of current vibrant directions, and explicate promising overlaps to adjacent fields such as quantum computation.

Wednesday 7th of June 2023

Superconductivity and Topology (9:00-12:50)

10:00-10:35

COLOSSAL ORBITAL EDELSTEIN EFFECT IN NONCENTROSYMMETRIC SUPERCONDUCTORS

Luca Chirolli

CNR Nanotec, Lecce, Italy

In superconductors that lack inversion symmetry, the flow of supercurrent can induce a nonvanishing magnetization, a phenomenon which is at the heart of nondissipative magnetoelectric effects, also known as Edelstein effects. For electrons carrying spin and orbital moments, a question of fundamental relevance deals with the orbital nature of magnetoelectric effects in conventional spin-singlet superconductors with Rashba coupling. Remarkably, we find that the supercurrent-induced orbital magnetization is more than 1 order of magnitude greater than that due to the spin, giving rise to a colossal magnetoelectric effect. The induced orbital magnetization is shown to be sign tunable and in the presence of superconducting phase inhomogeneities, a modulation of the Edelstein signal appears on the scale of the superconducting coherence length, leading to domains with opposite orbital moment orientations. The orbital-dominated magnetoelectric phenomena, hence, have clear-cut marks for detection both in the bulk and at the edge of the system and are expected to be a general feature of multiorbital superconductors with inversion symmetry breaking.

Wednesday 7th of June 2023

Superconductivity and Topology (9:00-12:50)

11:05-11:40 – Keynote

SUPERCONDUCTIVITY INDUCED BY THE INTERVALLEY COULOMB SCATTERING IN A FEW LAYERS OF GRAPHENE

Tommaso Cea

University of l'Aquila, Italy

We study the intervalley scattering induced by the Coulomb repulsion as a purely electronic mechanism for the origin of superconductivity in a few layers of graphene. The pairing is strongly favored by the presence of van Hove singularities in the density of states. We consider three different heterostructures: twisted bilayer graphene, rhombohedral trilayer graphene, and Bernal bilayer graphene. We obtain trends and estimates of the superconducting critical temperature in agreement with the experimental findings, which might identify the intervalley Coulomb scattering as a universal pairing mechanism in a few layers of graphene.

Wednesday 7th of June 2023

Superconductivity and Topology (9:00-12:50)

11:40-12:15

HIGH-THROUGHPUT SEARCH FOR NOVEL LOW-DIMENSIONAL SUPERCONDUCTORS FOR ALL-VDW TRANSMON QUBITS

Davide Campi

University of Milano Bicocca, Italy

The creation of a large-scale, fault-tolerant quantum computer would revolutionize many fields of science and economy enabling us to tackle in few seconds problems that would take thousands of years to solve on the largest classical supercomputer. Currently, the most technologically mature candidate as the core building block of such machines is the transmon qubit based on superconductor-insulator-superconductor interface known as Josephson junctions. The quality of this interface is key for the device performances but a sufficient quality can be hardly achieved with the conventional materials used in today's devices. Van der Waals (vdW)-bonded two-dimensional materials on the other hand are natural candidates to form atomically precise interfaces. Here we present the first results of a computational high-throughput search aimed at finding the best vdW-bonded low-dimensional superconductors for the realization of a future generation of all-vdW transmon qubits.

Wednesday 7th of June 2023

Superconductivity and Topology (9:00-12:50)

12:15-12:50

WEAK ERGODICITY BREAKING IN JOSEPHSON-JUNCTION ARRAYS

Angelo Russomanno

Scuola Superiore Meridionale, Naples, Italy

We study the quantum dynamics of Josephson-junction arrays. We find isolated groups of low entanglement eigenstates that persist even when the Josephson interaction is strong enough to destroy the overall organization of the spectrum in multiplets, and a perturbative description is no longer possible. These eigenstates lie in the inner part of the spectrum, far from the spectral edge, and provide a weak ergodicity breaking, reminiscent of the quantum scars. Due to the presence of these eigenstates, initializing with a charge-density-wave state, the system does not thermalize and the charge-density-wave order persists for long times. Considering global ergodicity probes, we find that the system tends toward more ergodicity for increasing system size: The parameter range where the bulk of the eigenstates look nonergodic shrinks for increasing system size. We study two geometries, a one-dimensional chain and a two-leg ladder. In the latter case, adding a magnetic flux makes the system more ergodic.

POSTERS

Session 1 – Monday 5th of June 2023 – 18:20-19:30

Filippo Bodo	*The Role of SOC-Induced Spin Currents on Weyl Semimetals and Topological Insulators*
Andrea Corradini	*Exploring the Phase Diagram of Silicon with Machine learning Potentials*
Jacopo Fiore	*Non-Linear Manipulation of Plasma Excitations in Cuprates with THz Light Pulses: from the Single- to the Bi-Layer Case*
Matteo Furci	*Light-Induced First Order Ferroelectric to Paraelectric Phase Transition in GeTe*
Francesco Macheda	*Dynamical screening of long-Range remote Electron-Phonon Coupling in Van der Waals Heterostructures*
Luca Maranzana	*Electric field driven Dynamics of Vortex Domain Walls in spiral Magnets*
Stefano Mocatti	*Light-induced non-thermal Phase Transition to the topological crystalline Insulator State in SnSe*
Alberto Pacini	*Accurate multiscale Simulation of frictional Interfaces by Quantum Mechanics/Green's Function molecular Dynamics*
Aditya Putatunda	*Interacting structural Orders and multiferroic Domains in $BaCoSiO_4$*
Paolo Restuccia	*High throughput first Principle Prediction of interfacial Adhesion Energies in Metal-on-Metal and Metal-Adsorbate-Metal Contacts*
Vittoria Urso	*Functionalization of 2D materials by intercalation.*
Lorenzo Varassi	*Quasiparticle and excitonic Properties of monolayer $SrTiO_3$*
Luciano Loris Viteritti	*Transformer variational Wave Functions for frustrated Quantum Spin Systems*

The Role of SOC-Induced Spin Currents on Weyl Semimetals and Topological Insulators

Filippo Bodo, Jacques K. Desmarais, and Alessandro Erba

Filippo Bodo

In recent years topological materials gained a lot of popularity in solid state physics due to their peculiar properties. They are a class of materials, insulators and semimetals, characterized by an exotic band structure where we can see the presence of Dirac, Weyl or Kane fermions. Therefore, these structures lead to properties that are of interest in the fields of spintronics, superconductivity and catalysis. In fact, topological materials can be either insulators or semimetals presenting only single points of contact between conduction and valence bands in the bulk, while being perfect conductors at the surface. A quantum-mechanical description of such materials is not trivial since their peculiar properties are often induced by the relativistic spin-orbit coupling (SOC) effect. In the context of density functional theory (DFT) simulations, it was recently shown that its generalization is needed for a proper account of such effects: the so-called spin current DFT (SCDFT). Even in absence of spin polarization, the SCDFT requires the dependence of the electron-electron potential on the the spin currents Jx, Jy and Jz, which was made possible only recently through the use of exact Fock exchange. Here we present the application of the SCDFT to the description of different topological materials: TaAs, a Weyl semimetal, and Bi (001) bilayer, a topological insulator.

Exploring the Phase Diagram of Silicon with Machine learning Potentials

Andrea Corradini, Giovanni Marini and Matteo Calandra

Andrea Corradini

The behaviour of undercooled liquid silicon has been long debated in literature. Various computational studies suggest the presence of a first-order phase transition between a high-density and a low-density liquid state in the undercooled domain, although very little experimental data is available to confirm or reject this hypothesis. In my research I am trying to fit machine learning interatomic potentials for silicon against a dataset of quantum-mechanical reference properties; the fitted potentials are then validated by running classical molecular dynamics simulations and used to characterise the undercooled liquid phase.
The long-term goal of this research is to extend this procedure to study photoexcited silicon: machine learning potentials fitted against a dataset of photoexcited configurations will be used to study how photoexcitation changes the phase diagram of silicon and whether it stabilizes new phases that were not obtainable in silicon under ordinary conditions.

ACKNOWLEDGEMENTS:
We acknowledge the financial support from the European Union ERC Project – 101052708 – DELIGHT

Non-Linear Manipulation of Plasma Excitations in Cuprates with THz Light Pulses: from the Single- to the Bi-Layer Case

J. Fiore, N. Sellati, F. Gabriele, M. Udina, G. Seibold, C. Castellani and L. Benfatto

Jacopo Fiore

In the past few years several groups observed an enhanced THz Third Harmonic Generation (THG) below the superconducting critical temperature of various cuprates. For in-plane polarized incoming fields the interplay between superconducting amplitude, quasiparticle and more exotic order-related collective excitations is still debated [1-4], with an even richer phenomenology than the one discussed in conventional superconductors [5-6]. However, when the field is c-axis polarized, it is accepted that non-linear excitation of the soft out-of-plane Josephson plasma mode (JPM) plays a crucial role. This has been experimentally established in single-layer La-based systems [7-9], where the THG signal is resonant when the central frequency of the pump matches ωJPM, and theoretically explained in a previous work [10]. Conversely, in bi-layer YBCO the experimental third harmonic kernel is monotonic in temperature even when the resonance condition between pump frequency and ωJPM is fulfilled [11]. Here, we will show how it is possible to explain both experimental findings invoking the same non-linear excitation process of two Josephson plasmons [12]. The crucial point is to consider the full momentum dispersion of the plasmon, which in anisotropic materials extends between the very different energy scales of in- and out-of-plane phase fluctuations, as measured e.g. by RIXS [13-14]. We ultimately obtain third harmonic kernels in the single- and bi-layer case which are in excellent agreement with the ones extracted from the experiments after a proper first harmonic normalization due to the reflection geometry.

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Light-Induced First Order Ferroelectric to Paraelectric Phase Transition in GeTe

Matteo Furci, Giovanni Marini, Matteo Calandra

Matteo Furci

GeTe represents the prototypical phase change material, conserving many potential applications despite its simple stoichiometry. The constrained density functional approach developed by Marini and Calandra [1] is used to detect the ultrafast photoinduced ferroelectric to paraelectric phase transition in GeTe. Harmonic phonon analysis finds the ferroelectric phase to be always the dynamically stable structure at any photoexcited electron concentrations considered. However, it is only through the non perturbative accounting of anharmonic effects in the description of the lattice dynamics that the expected stabilization of the cubic structure is observed upon photoexcitation. The photoinduced phase transition is identified to be of the first order and a convenient picture to interpret the experimentally available time resolved diffraction spectra is proposed. This work paves the way to the application of quantum anharmonic effects to ultrafast photoinduced structural phase transitions in phase change materials.

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Dynamical Screening of long-Range remote Electron-Phonon Coupling in Van der Waals Heterostructures

Francesco Macheda, Thibault Sohier and Francesco Mauri

Francesco Macheda

Van der Waals heterostructures are a versitale tool in order to enhance or induce unusual properties in a 2D target layer embedded in an fine-tuned dielectric environment. We introduce a general framework which makes use of ab initio calculations and semianalytical models to compute the long-range remote coupling between the dielectric environment and the target layer, with the inclusion of dynamical (non-adiabatic) effects. Taking into account plasmon-phonon hybridization, the dynamically screened remote electron-phonon interactions result to be strongly enhanced in the low doping regime, with a consequent change of regime in the target layer resistivity.

ACKNOWLEDGEMENTS
F. Macheda and F. Mauri acknowledge the financial support from the European Union ERC-SYN MORE-TEM No 951215.

Electric field driven Dynamics of Vortex Domain Walls in spiral Magnets

L. Maranzana and S. Artyukhin

Luca Maranzana

Domain wall motion is one of the most compelling problems in spintronics because it is the mechanism underlying the magnetization switching. The majority of existing information storage devices (e.g. hard drives) use a magnetic field for recording, which implies a considerable power consumption and limits the information density. Multiferroics hold promise for allowing magnetization control by an electric field. In type-II magnetoelectric multiferroics, the magnetic order breaks inversion symmetry and induces a ferroelectric polarization. The paradigmatic example is a spiral magnet. The domain wall between two spiral domains with opposite chirality generally consists of a periodic chain of vortices or merons. Here we study the electric field driven dynamics of vortex domain walls in cycloidal spiral magnets. We derive an analytical expression for the domain wall structure in the Ginzburg-Landau framework and apply the collective coordinates approach to formulate its dynamics in terms of soft modes. We solve the equations of motion and corroborate the results with atomistic spin dynamics simulations. We also discuss the dimerization of the vortex chain that occurs at high fields and possible breakdown scenarios.

Light-induced non-thermal Phase Transition to the topological crystalline Insulator State in SnSe

Stefano Mocatti, Giovanni Marini, Matteo Calandra

Stefano Mocatti

Femtosecond pulses can be used to reveal hidden broken symmetry states. However, these states are mostly transient and disappear after the laser removal. Photoinduced phase transitions towards crystalline metastable states are rare. Here, by using constrained density functional perturbation theory and accounting for light-induced quantum anharmonicity, we show that ultrafast lasers can permanently transform the topologically-trivial orthorhombic structure of SnSe into the topological crystalline insulating rocksalt phase via a first-order non-thermal phase transition. We describe the reaction path and evaluate the critical fluence. Our simulations of the photoexcited

structural and vibrational properties are in excellent agreement with recent pump-probe data in the low fluence regime below the transition, demonstrating the high accuracy of our theoretical framework.

ACKNOWLEDGEMENTS:
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Accurate multiscale Simulation of frictional Interfaces by Quantum Mechanics/Green's Function molecular Dynamics

Seiji Kajita, Alberto Pacini, Gabriele Losi, Nobuaki Kikkawa and Maria Clelia Righi

Alberto Pacini

Understanding frictional phenomena is a fascinating fundamental problem with huge potential impact on energy saving. Such an understanding requires monitoring what happens at the sliding buried interface, which is almost inaccessible by experiments. Simulations represent powerful tools in this context, yet a methodological step forward is needed to fully capture the multiscale nature of the frictional phenomena. Here, we present a multiscale approach based on linked ab initio and Green's function molecular dynamics, which is above the state of-the-art techniques used in computational tribology as it allows for a realistic description of both the interfacial chemistry and energy dissipation due to bulk phonons in non-equilibrium conditions. By considering a technologically relevant system composed of two diamond surfaces with different degrees of passivation, we show that the presented method can be used not only for monitoring in real time tribolochemical phenomena such as the tribologically-induced surface graphitization and passivation effects but also for estimating realistic friction coefficients. This opens the way to in silico experiments of tribology to test materials to reduce friction prior to that in real labs.

Interacting structural Orders and multiferroic Domains in $BaCoSiO_4$

Aditya Putatunda, Sergey Artyukhin

Aditya Putatunda

Unraveling the interdependence of ferroic orders in type II multiferroics enables new functionalities and devices. The symmetries present in a system play an important role in bringing forth the plausible cross-functionalities of such a multiferroic, where, for instance, electric field can be used to manipulate the magnetic moments or vice versa. Here we present our symmetry analysis and first-principles results on the novel chiral magnet $BaCoSiO_4$ which shows multiple ferroic characters like structural chirality, ferroelectricity and antiferromagnetism. Recent studies have reported the field tunability of chiral toroidal moments along with an exotic magnetoelectric effect where the resulting polarization is perpendicular to the applied field. The proposed phenomenological Landau-type theory, combined with density functional theory calculations predicts the energetics of the various phases and peculiar composite domain walls.

High Throughput first-Principle Prediction of interfacial Adhesion Energies in Metal-on-Metal Contacts

Paolo Restuccia, Gabriele Losi, Omar Chehaimi, Margherita Marsili, Maria Clelia Righi

Paolo Restuccia

Adhesion energy, a measure of the strength by which two surfaces bind together, ultimately dictates the mechanical behaviour and failure of interfaces. As natural and artificial solid interfaces are ubiquitous, adhesion energy represents a key quantity in a variety of fields ranging from geology to nanotechnology. However, researchers and engineers still rely on qualitative "compatibility" tables regarding adhesion in solid interfaces. An ab initio determination of adhesion energies is crucial because the specific atomistic details of the interface primarily determine the strength of adhesion. The atomistic simulation of heterogeneous interface is nevertheless challenging, as computations can quickly become very expensive. We developed a software, TribChem [1], a modular scientific workflow connected to publicly available databases, and performed the high-throughput ab initio screening of the adhesion energy of around a hundred metallic heterostructures, ranging from transition to noble metals [2]. The dataset allowed us to identify general trends confirming a correlation of interfacial adhesion and electronic charge already observed for homogeneous interfaces [3,4]. Finally, by using a machine learning approach, we obtained a simple analytical expression for predicting the adhesion energy from the surface energy and other intrinsic properties of the two heterostructure constituents alone, which can prove useful for avoiding expensive supercell calculations.

ACKNOWLEDGEMENTS
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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Functionalization of 2D materials by intercalation

Vittoria Urso

Alkali metals (AM) intercalate into graphite leading to the formation of AM-graphene layered materials (with AM = Li, Na, K, Rb, Cs). Intercalated species can modify the very electronic structure of graphene and consequently its electron mobility. Open question is how AM interact on graphene depending on the structure and coverage. We want to tackle this issue by first-principle calculations, in particulary density funzional theory, starting from a prototype system like K-graphene in different structural configurations and atomic percentages. Calculations are

performed within first-principles DFT (density functional theory) under the local density approximation LDA. The QUANTUM ESPRESSO package is used to perform all calculations; codes in the package are based on density functional theory and on a plane wave/pseudopotential description of the electronic ground state and are ideally suited for structural optimizations (both at zero and at finite temperature), linear response calculations (phonons, elastic constants, dielectric and Raman tensors, etc.) and high-temperature molecular dynamics. Calculations for (2×2) and (4×4) pristine undoped graphene, and (2×2) and (4×4) K-adsorbed on graphene are performed with the same-sized hexagonal supercell. In particular, we analyze three different structural configurations: (i) K on one side, (ii) K on alternate sides, (iii) K between two graphene layers. The Brillouin zone is sampled with a 8×8×1 Γ centered k-point grid, and Gaussian smearing with a width of $\sigma = 0.01$ eV is used for the occupation of the electronic levels. The computational results predict a shift of the Dirac cone, which is qualitatively confirmed by UV photoelectron spectroscopy; the most significant observation is the progressive occupation of the pi* states shifted below the Fermi level EF, upon K adsorption. Further analysis is currently under study.

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Quasiparticle and excitonic Properties of monolayer $SrTiO_3$

Lorenzo Varrassi, Peitao Liu and Cesare Franchini

Lorenzo Varassi

Strontium titanate SrTiO3 is one of the most studied and paradigmatic transition metal oxides. Recently, a breakthrough has been achieved with the fabrication of freestanding SrTiO3 ultrathin films down to the monolayer limit. However, the many-body effects on the quasiparticle and optical properties of monolayer SrTiO3 remain unexplored. Using state-of-the-art many-body perturbation theory in the GW approximation combined with the Bethe-Salpeter equation, we study the quasiparticle band structure, optical and excitonic properties of monolayer SrTiO3. We show that quasiparticle corrections significantly alter the band structure topology; however, the widely used diagonal G0W0 approach yields unphysical band dispersions. The correct band dispersions are restored only by taking into account the off-diagonal elements of the self-energy. The optical properties are studied both in the optical limit and for finite momenta by computing the electron energy loss spectra. We find that the imaginary part of dielectric function at the long wavelength limit is dominated by three strongly bound excitonic peaks and the direct optical gap is associated to a bright exciton state with a large binding energy of 0.93 eV. We discuss the character of the excitonic peaks via the contributing interband transitions, and reveal that the lowest bound excitonic state becomes optical inactive for finite momenta along γ, while the other two excitonic peaks disperse to higher energies and eventually merge for momenta close to M.

Transformer variational Wave Functions for frustrated Quantum Spin Systems

Luciano Loris Viteritti, Riccardo Rende, Federico Becca

Luciano Loris Viteritti

The Transformer architecture has become the state-of-art model for natural language processing tasks, avoiding recurrent and convolutional structures. Its key feature is the ability to describe long-range correlations among the elements of the input sequences. This approach has also been adapted to computer vision tasks, thus defining the Vision Transformer (ViT) architecture, obtaining competitive results compared to state-of-art deep Convolutional-Neural Networks. Motivated by these achievements, we propose an adaptation of the ViT architecture with complex parameters to define a new class of variational neural-network states for quantum many-body systems, the ViT wave function. We apply this idea to the one-dimensional J1-J2 Heisenberg model, demonstrating that a relatively simple parametrization gets excellent results for both gapped and gapless phases. In particular, the ViT state accurately describes exponentially decaying spin-spin correlations and the emergence of dimer order in the former case, as well as long-range spin-spin correlations within the latter one. The success of the ViT wave function relies on mixing both local and global operations, thus enabling the study of large systems with high accuracy.

Session 2 – Tuesday 6th of June 2023 – 17:45-19:30

Nearest-Neighbor Entanglement across the Mott-Hubbard Transition

G. Bellomia, C. Mejuto-Zaera, A. Amaricci, M. Capone

Gabriele Bellomia

The fast developing field of quantum information theory has greatly influenced the latest research in many-body physics. New perspectives on metal-insulator transitions in strongly correlated systems have recently emerged [1–4], inspired by novel cold-atom experiments able to estimate the entanglement and mutual information between a local site and its environment [5]. Unfortunately, these single-site quantities include on equal footing correlations for all spatial ranges in the system, making it difficult to gain physical insight besides reproducing the phase diagram. Using state-of-the-art cluster dynamical mean-field theory, we provide an alternative depiction of the Mott transition in terms of suitably defined bond quantities: through them we estimate the genuine quasilocal entanglement between a pair of neighboring lattice sites, with no contribution from the simulated environment. In the Mott insulator, the nearest-neighbor mutual information is shown to be resilient to local parity and particle number superselection rules, which have been recently proposed to be the hallmark for a faithful definition of operationally available entanglement in condensed matter systems [6,7].

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Polaronic Phases in Vanadium Trihalides

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Two dimensional (2D) van der Waals transition metal trihalides are a new class of functional material showing exotic physical properties and intrinsic 2D magnetism. Since the discovery of 2D intrinsic magnetism in Cr-based compound (https://doi.org/10.1038/nature22391), exotic magnetic phases, topological and chiral states (https://doi.org/10.1103/PhysRevLett.128.177202) stimulated the research in this field. Nowaday Vanadium trihalides (VX_3, X=Cl,Br,I) have been successfully syntetized and are currently studied. Indeed, the electronic ground state of these compounds is determined by the complex interplay between crystal field effects, electronic correlation, spin-orbit coupling, structural distorsion and mixed valence (10.1039/C9CP05643B). As a proof of this, we recently enrich the physics of Vanadium trihalides by discovering polaronic phases (arXiv:2301.06501) that explains apparently contradictory experimental evidences (https://doi.org/10.1021/acs.nanolett.2c04045, https://doi.org/10.1021/acs.nanolett.2c01922, https://doi.org/10.1063/5.0108498). These 2D polarons could be tuned by external doping or pumping with radiation and will strongly affect the 2D magnetism of these compounds.

Superconductivity induced by the Intervalley Coulomb scattering in a few Layers of Graphene

Tommaso Cea

We study the intervalley scattering induced by the Coulomb repulsion as a purely electronic mechanism for the origin of superconductivity in a few layers of graphene. The pairing is strongly

favored by the presence of van Hove singularities in the density of states. We consider three different heterostructures: twisted bilayer graphene, rhombohedral trilayer graphene, and Bernal bilayer graphene. We obtain trends and estimates of the superconducting critical temperature in agreement with the experimental findings, which might identify the intervalley Coulomb scattering as a universal pairing mechanism in a few layers of graphene.

Absence of Electron-Phonon-mediated Superconductivity in Hydrogen-intercalated Nickelates

Simone Di Cataldo, Paul Worm, Liang Si, Karsten Held

Simone Di Cataldo

The recently discovered nickelate superconductors represent one of the raising hot topic in the research area of strongly-correlated superconductors. A recent experiment [X. Ding et al., Nature 615, 50 (2023)] indicates that superconductivity in nickelates is restricted to a narrow window of hydrogen concentration: $0.22 < x < 0.28$ in $Nd_{0.8}Sr_{0.2}NiO_2H_x$. This reported necessity of hydrogen suggests that it may play a crucial role for superconductivity, as it does in the vast field of hydride superconductors, by boosting the electron-phonon coupling and hence a source of conventional superconducting pairing. Using density-functional theory and its extensions, we explore the effect of topotactic hydrogen on the electronic structure and phonon-mediated superconductivity in nickelate superconductors. Our calculations show that the electron-phonon coupling in hydrogen-intercalated nickelates is not strong enough to drive the electron pairing, and thus cannot explain the reported superconductivity.

Quantum Transport through spintronic Nano-Devices

Andrea Droghetti

I will present our work related to the development of theoretical and computational methods to simulate spintronic devices from first-principles. I will first review the combination of Density Functional Theory (DFT) with the non-equilibrium Green's functions (NEGF) method [1]. In particular, I will explain how we tailored DFT+NEGF to compute spin currents [2] and (out-of-equilibrium) magnetic moments in materials thus estimating effects such as spin transfer torque and current-induced spin polarization [3]. I will then describe how DFT+NEGF is further combined with Dynamical Mean Field Theory (DMFT) [4, 5] to treat electron correlation beyond a static mean-field picture. The method can be readily applied to solid-state heterostructures, such as Co/Cu /Co or Fe/MgO/Fe, accurately capturing effective mass renormalization as well as non-coherent effects in the 3d bands of transition metals [6, 7].

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Single-Point Spin Chern Number for disordered two-dimensional topological Insulators

R. Favata and A. Marrazzo

Roberta Favata

We present an approach for the calculation of the topological invariant in non-crystalline two-dimensional quantum spin Hall insulators [1]. The introduction of disorder breaks the translational symmetry and implies the use of large simulation cells, where the k-point sampling is typically reduced to the single Gamma point. We introduce a single-point formula for the spin Chern number that enables to study disordered quantum spin Hall insulators within the supercell framework. Inspired by the work of Prodan [2] our approach works even when the spin operator Sz does not commute with the Hamiltonian, as in the presence of Rashba spin–orbit coupling. We validate our method on the Kane-Mele model, both pristine and in presence of Anderson disorder. Then, we investigate the disorder-driven transition from a trivial to a topological phase known as topological Anderson insulator. Finally, we leverage the Wannier-function formalism and deploy our method with ab initio tight-binding Hamiltonians.

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Exploring electronic Properties of Phase-Change Arsenic Telluride

Pietro Maria Forcella

Pietro Maria Forcella

Arsenic Telluride, As_2Te_3, is a layered van der Waals semiconducting material known for its thermoelectric properties and structural phase transitions. The polymorfism of As_2Te_3 in pressure and temperature combined with its electronic and thermal properties make it an interesting phase-change material for future devices. Here, we studied the electronic properties of the α, β and β' phases by using angle-resolved photoemission spectroscopy (ARPES) and density-functional theory (DFT). In addition to the spectroscopic signature, we were able to isolate in α- As_2Te_3 anisotropic 2D electronic states, decoupled from the electronic structure, that we propose to ascribe to single layer (SL) β-tellurene. β-tellurene is a semiconducting monolayer that combines air stability, high room-temperature mobility, and low thermal conductivity which has been difficult to experimentally access otherwise.

Mott Enhanced Exciton Condensation

S. Giuli, A. Amaricci, M. Capone

Samuele Giuli

An Exciton Condensate is an elusive phase of insulating matter with increasing evidence coming from experiments on Quantum Wells, Quantum Hall Bilayers, Graphene and more recently also TMDs heterostructures. The latter materials are under the spotlights being a versatile platform to study many unconventional phenomena like Mott transition. Using Dynamical Mean Field Theory we have show that Mott physics plays a role in stabilizing the excitonic condensate phase by means of Mott localization of excitons. We computed the zero temperature phase diagram for a paradigmatic two orbital model showing that, in the vicinity of the Mott insulating phase, the Exciton Condensate phase is enlarged and this enlargement is connected with an increase in the number of local incoherent electron-hole pairs and a reduction of the spatial extension of the exciton.

Unveiling the Symmetry of the Pairing in the superconducting Sn/Si via intense electromagnetic Excitation

Mattia Iannetti, Tommaso Cea and Gianni Profeta

Mattia Iannetti

The α-phase of Sn/Si(111) has been studied for quite a long time with evidences of strong correlations and frustrated antiferromagnetic magnetism. Only recently, superconductivity has been reported in the hole-doped regime, with a critical temperature of $\sim$ 4.7 K [1,2]. However, the pairing mechanism and the symmetry of the superconducting (SC) order parameter are still under debate [2,3]. In this work we investigate the response of the SC Sn/Si to an intense electromagnetic (em) field. Assuming that the pairing is induced by the antiferromagnetic correlations, we describe the unperturbed SC state within the t−J model in the triangular lattice. The dynamics induced by the em perturbation is tracked by studying the precession of the Anderson's pseudo spins, which is equivalent to solving the Bloch's equations non-perturbatively. Using realistic parameters, we obtain a nematic d-wave superconductivity in the absence of the em field. Next, we introduce an intense THz em pulse and calculate the resulting third-harmonic-generation (THG) as a function of the polarization of the incident field. As a consequence of the nematic nature of the SC pairing, we find that the THG exhibits a minimum period of π, in contrast to the period of $\pi/3$ expected for pure s-wave pairing. In conclusion, our study shows that the polarization-dependent THG measured in a THz pump experiment can unveil the symmetry of the SC order parameter in the α-phase of Sn/Si(111).

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Born effective Charges and vibrational Spectra in super and bad conducting Metals

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Guglielmo Marchese

Vibrational spectroscopy in metallic systems. A new interest in employing Infra-Red Spectroscopy (IRS) for studying vibrational properties in metals aroused in the last decades (and even more in the last months) because there exist a variety of systems whose properties guarantees simultaneously the necessity of this technique and its feasibility. They are called "super-Hydrides" andare particularly renown for manifesting a superconducting phase at very high-temperature under ultra-high pressure (UHP). I would present the ab-initio DFT approach and the computational strategy I adopted to simulate the H3S spectrum published in Capitani et al., Nat. Phys. (2017). Although vibrational spectroscopy is commonly prevented in metals, the super-hydrides are not the only systems where this technique gives access to structural properties. It is sufficient that the intense electronic response that characterized the low-energy spectrum of metals does not obliterate the other features in the region. A small free-carriers density or a short electronic lifetime (due for example to a strong electron-phonon coupling), may hinter the electronic response enough for the vibrational and thestructural signature of the material to become experimentally accessible. A strong electron-phonon interaction is the property that allow the high-Tc BCS superconductivity of super-Hydrides. Moreover, the UHP apparatus prevents most techniques for sample characterization except IRS, making super-Hydrides perfect candidates for this measurement.

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Multipartite Entanglement in the Measurement-Induced Phase Transition of the Quantum Ising Chain

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External monitoring of quantum many-body systems can give rise to a measurement-induced phase transition characterized by a change in behavior of the entanglement entropy from an area law to an unbounded growth. We show that this transition extends beyond bipartite correlations to multipartite entanglement. Using the quantum Fisher information, we investigate the entanglement dynamics of a continuously monitored quantum Ising chain. Multipartite entanglement exhibits the same phase boundaries observed for the entropy in the post-selected no-click trajectory. Instead, quantum jumps give rise to a more complex behavior that still features the transition, but adds the possibility of having a third phase with logarithmic entropy but bounded multipartiteness.

Structural Relaxation by Means of Ab initio Molecular Dynamics: Development and Implementation in the CRYSTAL Code

Chiara Ribaldone, Silvia Casassa

Chiara Ribaldone

Structural optimization is the necessary starting point for an ab initio study of the ground state properties of materials, such as electronic, vibrational or optical ones. This procedure consists in minimizing the energy of an atomic structure, finding a local minimum in the potential energy surface (PES) which describes the energy of an atomic system as a function of its configuration state. A very well established and commonly used optimization method is a quasi-Newton line-search algorithm, based on an approximation of the Hessian matrix and on its updating at each minimization step by means of the Broyden-Fletcher-Boldfarb-Shanno (BFGS) formula. At the same time, recent works have highlighted that the so-called Fast Inertial Relaxation Engine (FIRE), an optimization methods based on Molecular Dynamics (MD) concepts, could be very efficient and even competitive with BFGS scheme. In the present work, we have implemented this novel FIRE structural optimization method in the CRYSTAL code, an ab initio quantum mechanical package for condensed matter simulations. The efficiency of FIRE algorithm has been assessed for different atomic systems with various dimensionality and kind of chemical bonding. This work could paved the way for further improvement of FIRE minimization algorithm in the CRYSTAL code, allowing to perform structural optimization at finite temperature or transition state calculations in conjunction with Nudged Elastic Band method.

Strain induced Changes in Surface and topological properties of $NiTe_2$ Dirac Semimetal

Paolo Settembri, Federico Mazzola, Gianni Profeta and Antonio Politano

Paolo Settembri

We investigate the topological surface states of $NiTe_2$ using DFT calculations. NiTe2 is a layered transition metal dichalcogenide (TMD), that has attracted interest in the scientific community, due to the presence of a type-II Dirac point near the Fermi level and the presence of band inversions along the Γ-A direction that lead to topological surface states. We analyze their dispersion and spin texture, comparing them with Arpes measurements, and using a novel experimental technique to study the effect of strain on their dispersion. Our study suggests the possibility of tuning $NiTe_2$'s topological surface states with strain for technological applications, like in spintronics.

Wigner Gaussian Dynamics: simulating the anharmonic and Quantum ionic Motion

Antonio Siciliano, Lorenzo Monacelli, Giovanni Caldarelli and Francesco Mauri

Antonio Siciliano

The atomic motion controls important features of materials, such as thermal transport, phase transitions, and vibrational spectra. However, the simulation of ionic dynamics is exceptionally

challenging when quantum fluctuations are relevant (e.g., at low temperatures or with light atoms) and the energy landscape is anharmonic. In this work, we formulate the Time-Dependent Self-Consistent Harmonic Approximation (TDSCHA) in the Wigner framework, paving the way for the efficient computation of the nuclear motion in systems with sizable quantum and thermal anharmonic fluctuations. Besides the improved numerical efficiency, the Wigner formalism unveils the classical limit of TDSCHA and provides a link with the many-body perturbation theory of Feynman diagrams. We further extend the method to account for the non-linear couplings between phonons and photons, responsible, e.g., for a nonvanishing Raman signal in high-symmetry Raman inactive crystals, firstly discussed by Rasetti and Fermi. We benchmark the method in phase III of high-pressure hydrogen ab initio. The nonlinear photon-phonon coupling reshapes the IR spectra and explains the high-frequency shoulder of the H2 vibron observed in experiments. The Wigner TDSCHA is computationally cheap and derived from first principles: it is unbiased by assumptions on the phonon-phonon and phonon-photon scattering and does not depend on empirical parameters. Therefore, the method can be adopted in unsupervised high-throughput calculations.

Charge-to-Spin Interconversion at (111) $LaAlO_3/SrTiO_3$ Interface

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Mattia Trama

Converting charge current into spin current is one of the main mechanisms exploited in spintronics. One prominent example is the Edelstein effect, namely, the generation of a magnetization in response to an external electric field, which can be realized in systems with lack of inversion symmetry. If a system has electrons with an orbital angular momentum character, an orbital magnetization can be generated by the applied electric field, giving rise to the so-called orbital Edelstein effect. Oxide heterostructures are the ideal platform for these effects due to the strong spin–orbit coupling and the lack of inversion symmetries. Beyond a gate-tunable spin Edelstein effect, we predict an orbital Edelstein effect an order of magnitude larger then the spin one at the (111) $LaAlO_3/SrTiO_3$ interface. We model the material as a bilayer of t_{2g} orbitals using a tight-binding approach, and show that the hybridization between the electronic bands crucially impacts the Edelstein susceptibility.

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