BOOK OF ABSTRACTS

ETSF Informal Meeting 2026

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September 7–10

CNR Hall, Via dei Taurini 19, Rome, Italy

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Chair: ***Giovanni Onida*** *(University of Milan)*

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Poster Session Abstracts

Poster #1: g-C6N6: A 2D Semiconductor with Dirac Cones & Flat Bands

Authors: Stefano Lista
Affiliation: University of Rome Tor Vergata

Abstract: The ongoing search for two-dimensional (2D) materials often aims to combine the exceptional charge carrier mobility of graphene with a finite bandgap, a crucial requirement for novel electronic and optoelectronic applications. This work presents a comprehensive first-principles study of g-C6N6 (graphitic heptazine-based carbon nitride), a 2D organic direct-gap semiconductor characterized by a porous Kagome-like lattice geometry. Through a rigorous computational approach combining Density Functional Theory (DFT), Density Functional Perturbation Theory (DFPT), and the Boltzmann Transport Equation (BTE), we investigate the structural, electronic, optical, vibrational, and transport properties of this material. Our electronic structure calculations reveal that g-C6N6 exhibits a direct bandgap at the K point of the Brillouin zone. Remarkably, the band structure hosts both highly dispersive Dirac cones in the conduction band (ensuring high carrier mobility) and nearly flat bands in the valence region, which promote electronic localization and strong many-body correlations. Optical property analysis using a scissor operator on the energy spectra based on the work of Liang et al. within an independent particle approach, supplemented by the Ritova-Keldysh potential model, uncovers an exceptionally large exciton binding energy of 2.96 eV. Furthermore, phonon dispersion calculations confirm the dynamical stability of the 2D lattice, with electron-phonon coupling found to be most intense for high-energy optical phonons. We investigate the intrinsic charge transport and ultrafast dynamics by evaluating band-projected scattering rates. Transport calculations indicate that carrier mobility at the Dirac cones reaches high values and is heavily dominated by acoustic phonon scattering. In stark contrast, mobility at the band edges (Conduction Band Minimum and Valence Band Maximum) is significantly suppressed. Consequently, at room temperature (300 K), carrier relaxation times at the band edges are drastically reduced to the order of a few femtoseconds. These findings establish g-C6N6 as a highly promising platform for exploring the interplay between high charge mobility and correlated quantum phases in 2D polymers.

Poster #2: Lead-Free Cs/Rb–Sn/Ge Halide Perovskites : Structure–Property Relationships and Phase-Stability

Authors: Giancarlo Cappellini, Claudio Ribeiro da Silva, Gianluca Gatto, Amit Kumar, Alessio Filippetti, Lara Kühl Teles, Marcelo Marques
Affiliation: University of Cagliari

Abstract: Lead-free halide perovskites have emerged as promising candidates to overcome the toxicity and sustainability limitations associated with Pb-based absorbers in next-generation photovoltaics. In this work, we present a systematic first-principles investigation of fully inorganic ABI3 compounds (A = Cs, Rb; B = Sn, Ge) as environmentally benign alternatives composed of earth-abundant and low-cost elements. Using a consistent ab-initio – DFT+DFT–½

framework including relativistic effects, we evaluate structural stability, band gaps, carrier effective masses, and optical properties across four families of polymorphs. Three-dimensional Sn- and Ge-based phases exhibit direct band gaps in the optimal photovoltaic window, strong absorption coefficients, and light ambipolar effective masses. This work establishes quantitative structure–property–stability relationships for lead-free Sn/Ge iodide perovskites and provides design guidelines toward low-cost, low-toxicity, and scalable photovoltaic materials.

Poster #3: Benchmark study of many-body methods for the prediction of band alignment at hetero-interfaces, using small Hubbard models. abstract in other form

Authors: Jean Goossaert
Affiliation: LSI, Ecole Polytechnique

Abstract: In a photovoltaic cell, a current is obtained by breaking photo-induced electron-hole pairs at a junction between an absorber and a transport layer. This separation is made possible by a proper offset of the electronic bands at the interface. Therefore, predicting this band offset with good precision is crucial for predicting the efficiency of the cell. Most many-body techniques however fail at reliably predicting the valence and conduction band offsets in agreement with experimental data [1]. In addition, discrepancies appear between the experimental values as well. Therefore, a benchmark study of the band alignment in various types of heterojunctions is needed. The approach presented in this talk is to start from the simplest model junction, the asymmetric Hubbard dimer, and study the range of validity of several many-body approximations in all possible regimes. This model has the great advantage to be exactly solvable, providing the exact addition/removal energies as a benchmark. In particular, results for exact Kohn-Sham DFT, Hartree-Fock and several GW flavors will be discussed. This study is then extended to a simple but more realistic interface relevant to photovoltaic applications.

References:
[1] A. Lorin, T. Bischoff, A. Tal, and A. Pasquarello, Phys. Rev. B 108, 245303 (2023)

Poster #4: First-Principles Raman Spectroscopy of Chalcogenide Perovskites and Polar Ternary Oxides

Authors: Rashmi Sharma
Affiliation: University of Luxembourg

Abstract: Chalcogenide perovskites are a very attractive material class for optoelectronics due to their excellent stability. The bandgap can be tuned by alloying of the chalcogen atoms, e.g., replacing parts of the sulfur atoms with selenium atoms. This alloying has an impact on the vibrational properties of the crystal and can be investigated by Raman spectroscopy. We investigate the phonons and Raman spectra of $BaZr(S_{1-x}Se_x)_3$ alloys for the whole compositional range (0 <= x <=1). To avoid the use of computationally expensive supercells, we calculate dynamical matrices for $BaZrS_3$ and $BaZrSe_3$ and mimic alloying by interpolation. Likewise, the anion masses are scaled (32<= m <=79amu). A visualization framework has been developed using the calculated Raman spectra and the web interface of the Phonon website (https://henriquemiranda.github.io/phononwebsite/phonon.html). The modes and associated

shifts in frequency can be seen clearly as a function of Se concentration. In the second part, we calculate Raman spectra of the polar ternary oxide $Zn_2Mo_3O_8$. We calculate the dependence of the Raman spectra on the scattering geometry (direction and polarization of incoming and outgoing light). We discuss the observed position dependence of the dominant peaks on the light direction and discuss the selection rules for parallel versus cross-polarization.

Poster #5: Robust Approximations for the Polarizability of Complex Materials with Applications to Layered Perovskites

Author: Ilayda Ashgar
Affiliation: LSI, École Polytechnique

Abstract: Organic perovskites have demonstrated significant potential for technological applications, particularly in photovoltaics. To investigate the optical properties of these systems - often composed of many atoms - approximations and computational strategies are required to reduce the cost of evaluating a key quantity: the dielectric function. In this work, I will introduce the types of systems we study and the properties of interest within an ab initio theoretical framework, including density functional theory (DFT) and many-body Green's function approaches. I will then present ideas for simplifying the evaluation of the dielectric function using a method that avoids explicit summation over empty bands.

Poster #6 Designing explicit functionals for the charge density in terms of a potential

Authors: Muhammed H. Güneş [1,2], Ayoub Aouina [3], Vitaly Gorelov[1,2], Matteo Gatti[1,2,4], Lucia Reining[1,2]
Affiliation: [1] LSI, CNRS, CEA/DRF/IRAMIS, École Polytechnique, Palaiseau, France, [2] European Theoretical Spectroscopy Facility (ETSF), [3] Research Center Future Energy Materials and Systems of the University Alliance Ruhr and Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University Bochum, Germany, [4] Synchrotron SOLEIL, France

Abstract: One of the most powerful strategies to address properties of real many-body systems is to incorporate data obtained for models, for example, to use data of the homogeneous electron gas in order to build the Local Density Approximation for the Kohn-Sham exchange-correlation potential. In the present work, we examine to what extent we can use model data to design functionals directly for observables of materials. In particular, we study different approximations for the charge density of real inhomogeneous materials expressed as a simple, explicit functional of a given Kohn-Sham potential, using as central building block the Lindhard density-density response function of the homogeneous electron gas. Our increasingly realistic set of approximations includes a fully near- sighted expression equivalent to the Thomas-Fermi approximation, functional Taylor expansions, and different approximations to the Connector Theory developed in [Aouina et al., npj Computational Materials 11, 242 (2025)]. In all cases, the charge density is obtained without ever solving the Kohn-Sham Schrödinger equation. Results for cubic Helium, a prototypical strongly inhomogeneous material, systematically improve with higher levels of approximation, indicating that this is a promising route to obtain expressions that are relatively simple to calculate and to analyze.

Workshop Presentation Abstracts

Auxiliary systems for observables

Speaker: Lucia Reining
Affiliation: LSI, CNRS/CEA/Ecole Polytechnique/Institut Polytechnique de Paris, Palaiseau, France

Abstract: The Kohn-Sham approach is one of the major ingredients that led to the huge success of Density Functional Theory. In essence, in this approach one determines the charge density of a system of interacting electrons from an auxiliary system of non-interacting particles with a suitably designed effective potential. In this talk, we will look at the Kohn-Sham approach from different points of view, discussing the reasons for its success, major approximation strategies, and, most importantly, exploring how the idea could be generalized to determine from an auxiliary system observables other than the charge density.

Functional theory of the occupied spectral density and solution of its dynamical Euler-Lagrange equations

Speaker: Andrea Ferretti
Affiliation: CNR - Istituto Nanoscienze (NANO)

Abstract: We address the problem of interacting electrons in an external potential by introducing the occupied spectral density as fundamental variable. First we formulate the problem using an embedding framework and prove a one-to-one correspondence between a spectral density and the local, dynamical external potential that embeds it into an open quantum system. Then, we use the Klein functional to define a universal functional of the spectral density, introduce a variational principle for the total energy, and formulate a non-interacting mapping suitable for numerical applications. The resulting equations, which involve local and dynamical potentials, are then solved by using the algorithmic inversion method based on a sum-over-poles to represent propagators. At variance with time-dependent density-functional theory, this formulation aims at studying charged excitations and electronic spectra with a functional theory, although possibly leading to accurate approximations for the total energy.

Direct and inverse photoemission spectra from the screened multichannel Dyson equation

Speaker: Arjan Berger
Affiliation: Toulouse University

Abstract: In this talk, I will present the screened multichannel Dyson equation for the simulation of both direct and inverse photoemission spectra from first principles. The multichannel Dyson equation couples two or more many-body Green's functions to describe the electronic structure of materials. In particular, it can model photoemission spectra by coupling the one-body Green's function with the three-body Green's function [1,2]. Unlike methods using only the one-body Green's function, our approach puts the description of quasiparticles and satellites on equal footing. We have proposed a multichannel self-energy that goes beyond GW and describes both electron-hole and particle-particle contributions. It yields the exact spectral functions for the Hubbard dimer at any interaction strength. I will show how the multichannel Dyson equation can be recast as a simple eigenvalue problem. The screened multichannel Dyson equation improves upon the standard multichannel Dyson equation by correctly including the screening of all particle-particle and electron-hole interactions due to the presence of the other electrons [3]. Using the example of bulk silicon, we demonstrate that the screened multichannel Dyson equation can capture the main features of the direct and inverse photoemission spectra. In particular, it captures the correct position of the silicon plasmon satellite, unlike standard many-body approaches such as GW, which strongly overestimates the binding energy of this satellite. I will also show that multichannel Dyson equations can be constructed to describe other types of spectroscopies such as absorption spectroscopy including double excitations [4] and Auger spectroscopy [5].

References:
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[2] G. Riva, P. Romaniello, J. A. Berger, Phys. Rev. B 110, 115140 (2024)
[3] P. Romaniello, J. A. Berger, arXiv:2603.27329 (2026)
[4] G. Riva, Th. Fisher, S. Paggi, J. A. Berger, P. Romaniello, Phys. Rev. B 111, 195133 (2025)
[5] P. Sellié, J. A. Berger, P. Romaniello, arXiv:2604.01085 (2026)

Gauge invariant derivation of the matter–only Hamiltonian

Speaker: Andrea Marini
Affiliation: CNR Istituto di struttura della materia (ISM)

Abstract: Enrico Fermi in 1932, used classical Gauss equation to derive the Coloumb density–density in- teraction from the longitudinal electro–magnetic potential, in a gauge–invariant way. In this work we extend the Fermi procedure to the transverse component of the vector potential. By using a fully quantistic canonical transformation we replace the transverse vector potential with a current– current and current–current–density interactions. The transformed Hamiltonian is, then, projected in the fermionic space providing a matter–only gauge respecting Hamiltonian. We discuss how this Hamiltonian provides the quantistic origin of the longitudinal–transverse splitting observed in phonons and other elemental excitations.

Studying the sources of bias of One body reduced density matrices from Quantum Monte Carlo in solids.

Speaker: Carlos Rodriguez Perez
Affiliation: LSI, Ecole Polytechnique

Abstract: The one body reduced density matrix (1RDM) is a many-body object without a classical equivalent. It tells us a lot about the degree of correlation in the system, particularly how electrons occupy the single particle states. We have computed this object with Quantum Monte Carlo techniques for two systems. First, we have benchmarked the accuracy of QMC-1RDMs and densities, comparing them with the exact solution of the Helium atom, allowing us to identify how the trial wave function biases the DMC-computed 1RDM. Most recently we have computed the 1RDM of the silicon crystal, where we are studying how we can remove finite size effects. For this we are developing suitable extrapolation techniques which allow us to obtain the thermodynamic limit 1RDM.

First-Principles Study of Electronic and Optical properties of Transition Metal Oxynitrides: The Role of Anion Ordering

Speaker: Ivan Marri and Sudha Priyanka Ganesapandian
Affiliations: University of Modena and Reggio Emilia

Abstract: ransition-metal oxynitrides (TMONs) are an emerging class of materials that combine the chemical stability of oxides with the superior electronic and catalytic properties of nitrides, making them promising candidates for energy conversion and environmental applications, particularly photocatalysis. The simultaneous incorporation of oxygen and nitrogen into the crystal lattice introduces an additional degree of freedom through the arrangement of O^{2-} and N^{3-} anions, referred to as anion ordering (AOR), which can profoundly influence the structural, electronic, and optical properties of these materials. In this work, we explore the role of AOR in selected TMONs by considering different anionic configurations with identical chemical composition. By combining Density Functional Theory (DFT) and Many-Body Perturbation Theory (MBPT), we systematically assess the impact of AOR on the structural, electronic, and optical properties relevant to photocatalytic performance. Our results reveal clear correlations between anion arrangement and the resulting optoelectronic properties, enabling the identification of the most promising anion-ordering configurations for visible-light-driven photocatalytic applications.
Project funded by the Ministry of University and Research as part of the PRIN 2022 project no. 2022PKW527.

How Composition Shapes Self-Trapped Excitons in Double Perovskites

Speaker: Simone Grillo [1], Offir Zachs [2], Umberto De Giovannini [3], Yehonadav Bekenstein [2], Angel Rubio [1,4], Ofer Neufeld [2]
Affiliations: [1] Max Planck Institute for the Structure and Dynamics of Matter (MPSD) and Center for Free-Electron Laser Science (CFEL),Hamburg.[2] Technion - Israel Institute of Technology Haifa, Israel.[3] Dipartimento di Fisica e Chimica - Emilio Segrè, Università degli Studi di Palermo, Italy.[4] Center for Computational Quantum Physics (CCQ), The Flatiron Institute, New York, USA

Abstract: Self-trapped excitons (STEs) are widely invoked to explain the large Stokes shifts and broad photoluminescence (PL) of perovskites, yet the microscopic mechanisms in lead-free double perovskites (DPs) is still debated [1-4]. In particular, it is still unclear how alloying and dopants govern exciton localization, lattice distortion, and radiative recombination. We combine linear-response optical spectroscopy and first-principles theory to investigate STEs in lead- free metal halide DPs nanocrystals Cs2BInCl6 (B = Na, K), with and without Sb doping. Experimentally, we find that alloying continuously tunes the PL from about 2.25 to 2.75 eV, while the absorption onset remains near 3.8 eV, only weakly affected by composition. On the other hand, strong emission is observed only in Sb-doped samples, pointing to a key role of the dopant in the recombination process. To validate the experiments, we perform many-body perturbation theory calculations (GW and Bethe-Salpeter equation) together with constrained-DFT simulations of excited-state lattice relaxation. We identify a STE state in the doped compounds and show that the large redshift between absorption and emission originates from lattice-driven renormalization of dopant-hybridized in-gap states. We show that Sb doping opens bright recombination channels and modifies the exciton from a more localized state in the pristine crystal to a more extended excitation prior to self-trapping. Alloying controls the strength and character of the exciton-phonon coupling: Na- and K-based compounds favor different lattice displacements, leading to strongly tunable PL despite nearly unchanged absorption. Lastly, our ab-initio theory predicts extremely strong PL polarization anisotropies that directly reflect the spatial anisotropy of the STE, depending on the B-site composition. Time-resolved measurements perfectly match the theory, providing first experimental fingerprints of the excitonic wavefunction in DP and its composition dependence.

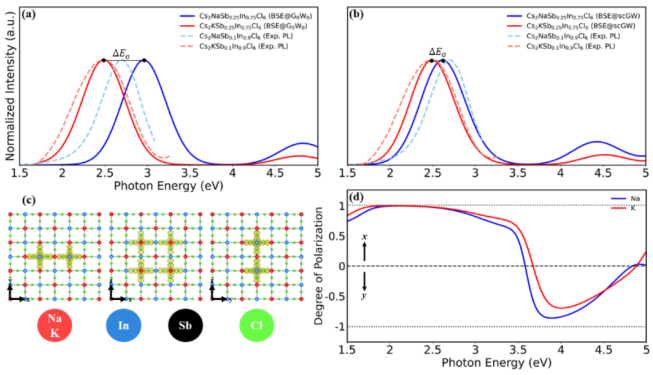

Figure 1

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[2] Noculak, Agnieszka, et al. Chemistry of Materials 32.12 (2020): 5118-5124.
[3] Gray, Matthew B., et al. Journal of Materials Chemistry C 8.20 (2020): 6797-6803.
[4] Cong, Muyu, et al. Science Bulletin 65.13 (2020): 1078-1084.

Perovskite Solar Cells and the impact of two-dimensional material on interface properties

Speaker: Aldo Di Carlo
Affiliations: CNR-ISM and University of Rome Tor Vergata, Rome

Abstract: Perovskite solar cells have emerged as one of the most promising photovoltaic technologies owing to their high power conversion efficiency, low-temperature processability, and compatibility with scalable fabrication. However, their performance and long-term operational stability remain strongly limited by interfacial losses, including non-radiative recombination, inefficient charge extraction, energy-level mismatch, ion migration, and defect-assisted degradation. In this context, two-dimensional materials have attracted increasing attention as powerful tools for interface engineering. In this talk I will highlight the impact of graphene and related two-dimensional materials, including MoS_2, graphene oxide, $Ti_3C_2T_x$ MXenes and 2D perovskites, on the tuning of interface properties in perovskite solar cells [1-5]. These materials can modify the electronic structure of charge transport layers, improve work-function alignment, passivate trap states, promote selective carrier extraction, and enhance the morphological and chemical stability of the perovskite absorber. Their atomically thin nature, high conductivity, tunable surface chemistry, and compatibility with solution processing make them particularly suitable for integration at the perovskite/electron transport layer and perovskite/hole transport layer interfaces. Furthermore, the use of two-dimensional materials has shown potential not only in small-area devices but also in large-area perovskite modules, supporting the transition from laboratory-scale efficiency toward industrially relevant stability and scalability. Overall, interface engineering based on two-dimensional materials represents a promising strategy to overcome the intrinsic limitations of perovskite solar cells and to accelerate their development into reliable next-generation photovoltaic technologies.

References:
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[2] S. Pescetelli, A. Agresti, G. Viskadouros. et al. Nature Energy 7, 597–607 (2022).
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[4] N. Yaghoobi Nia, M. Zendehdel et al. Nature Energy 11, 135–149 (2026)
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At the Interface: The Heart of Photoconversion Mechanisms

Speaker: Giacomo Giorgi
Affiliations: University of Perugia

Abstract: Interfaces between distinct chemical and structural species play a decisive role in determining the efficiency and pathways of photoconversion processes. Here we employ first-principles calculations to investigate the electronic structure, charge-transfer dynamics, and interfacial recombination channels of model heterostructures comprising oxide, molecular, and semiconductor components. Density functional theory (DFT), combined with many-body corrections where needed, is used to quantify band alignment, exciton binding energies, and non-radiative decay rates at representative interfaces. We show how local structural motifs, defect states, and interfacial dipoles modulate carrier separation and stabilization, and identify design principles—such as tailored chemical termination and controlled defect engineering—that optimize photogenerated charge extraction. Our atomistic insights link microscopic interfacial properties to macroscopic photoconversion performance and provide predictive guidance for the rational design of advanced photoactive materials and device architectures

Dehydration-initiated pathways for the boehmite-to-corundum transformation from first principles

Speaker: Giuliana Materzanini [1,2], Célia Dieudonné [3], Erwan Peigney [3], Angéline Poulon-Quintin [3], Marjorie Cavarroc [4], Cyril Aymonier [3], Gian-Marco Rignanese [1,5]
Affiliations: [1] Institute of Condensed Matter and Nanosciences (IMCN), Université catholique de Louvain, Louvain-la-Neuve, Belgium. [2] Institute of Mechanics, Materials and Civil Engineering (IMMC), Université catholique de Louvain, Louvain-la-Neuve, Belgium. [3] ICMCB, CNRS, Université de Bordeaux, Bordeaux INP, Pessac, France. [4] SAFRAN Tech, Châteaufort, France. [5] WEL Research Institute, Wavre, Belgium.

Abstract: The transformation of boehmite, γ-AlO(OH), into corundum, α-Al_2O_3, is a solid-state reconstruction governed by dehydration, water activity, and lattice rearrangement. Hydrothermal experiments have shown that α-Al_2O_3 formation from boehmite-based precursors is highly sensitive to water properties, especially density and water activity, which are controlled by pressure, temperature, and water content [1,2]. Motivated by this picture, we use first-principles simulations to disentangle two successive steps of the transformation: the initiation of dehydration in boehmite and the reconstruction of the resulting dehydrated structure into α-Al O . Ab initio molecular dynamics is used to compare pristine and partially dehydrated boehmite under thermal fluctuations. While temperature alone mainly induces orientational disorder of OH groups, removing a small number of H–OH pairs activates proton mobility within the hydrogen-bond network, triggering hydrogen transfer and making different dehydration motifs dynamically accessible. This suggests why low water density can promote further water expulsion, while re-hydration at higher density can quench the process. We then construct a commensurate pathway between dehydrated boehmite and corundum, and compute its minimum-energy path at the DFT level. The pathway reveals two coupled stages: lattice distortion with changes in Al coordination, followed by Al migration between adjacent layers, which completes the reconstruction of the corundum framework. This work shows how AIMD and minimum-energy-path calculations can translate a complex hydrothermal synthesis problem into a microscopic picture of proton mobility, lattice reconstruction, and phase stability.

References:
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DFT-molecular dynamics investigation on the Raman spectra of liquid water

Speaker: Taras Bryk [1], Rodolphe Vuilleumier [2] and Ari Paavo Seitsonen[2]
Affiliations: [1] Yukhnovskii Institute for Condensed Matter Physics of NAS of Ukraine & Lviv National Polytechnic University, 79013 Lviv, Ukraine, [2] École Normale Supérieure, Paris

Abstract: Water is an ubiquitous liquid that has several exotic and anomalous properties. Despite its apparent simple chemical formula, its capability of forming a dynamic network of hydrogen bonds leads to a rich variety of physics. Here we study the vibrations of water using molecular dynamics simulations, mainly concentrating on the Raman and infra-red spectroscopic signatures [1], using the Density Functional Theory as the engine to yield the forces between the atoms. We investigate the consequences of the varying temperature on the vibrational frequencies, and we enter the details of the hydrogen bonding coordination by using restrained simulations in order to gain quantitative insight on the dependence of the frequencies on the neighbouring molecules. Further we also explore the collective vibrational excitation modes in the liquid water [2] using machine learning interaction potentials, and we discuss the importance of the inclusion of the long-range Coulomb interactions in the learning.

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Time-resolved Raman spectroscopy in photoexcited MoS_2: transient doping, resonance effects and electron-phonon coupling

Speaker: Claudia Fasolato
Affiliations: University of Rome La Sapienza

Abstract: Graphene-like, layered materials are attracting increasing attention because of their potential in optoelectronics and in novel quantum technologies, given their electronic properties are often strongly influenced by dimensionality, offering an easy experimental knob for tunability [1]. A popular example is the indirect-to-direct bandgap transition occurring in transition metal dichalcogenides (TMDs) when they are exfoliated down to a single layer system. Unravelling the relaxation pathways of photoexcited electrons in quasi-2D systems and, specifically, their coupling to the lattice degrees of freedom, is of great applicative interest. Experimentally, time-resolved spontaneous Raman spectroscopy (TRRS) can provide direct access to the electron-phonon coupling dynamics, as well as the incoherent phonon relaxation, in the sub-ps timescale [2]. We have studied the deexcitation dynamics of MoS2 after impulsive optical pumping of the excitonic bandgap. At the SPRINT-NFFA facility, we have carried out a TRRS study on the system, monitoring the temporal evolution after photoexcitation of the Raman active features: the out-of-plane A1g mode, the in-plane E'2g mode, and a two-phonon feature associated with zone-edge acoustic modes. Equilibrium Raman spectroscopy studies have linked the modification of such phonon lineshapes to doping effects, providing the background for studying the optically induced, transient doping of the system [3,4,5]. We explore the effect of dimensionality on the system relaxation dynamics, by comparing the results on bulk and monolayer MoS2, revealing significant differences in the phenomenology and relaxation timescales [6]. We further show that a TRRS investigation on WS2 reveals a similar qualitative behavior, with significant differences in the specific timescales. After presenting our TRRS results, I will discuss their perspective integration in multi-messenger, time-resolved spectroscopy studies, coupling the time resolved photon and electron spectroscopies available at the SPRINT-NFFA facility (CNR-IOM@Elettra, Trieste, Italy).

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A Quantum Embedding Framework for Molecular Response Properties in Condensed Phase

Speaker: Alberto Barlini[1], Tommaso Giovannini [2]
Affiliations: [1] Scuola Normale Superiore di Pisa, [2] Università di Roma Tor Vergata

Abstract: Molecular response properties are central to the interpretation and design of functional systems for photonics, sensing, and nonlinear optical applications, yet their accurate description in the condensed phase remains challenging.[1–4] In such complex systems, the target molecule interacts with an environment ranging from transparent media, such as liquid solutions, to nanostructured substrates, such as metal nanoparticles.[1–4,6,8] A convenient route to address this complexity is to resort to quantum embedding methods, in which the full system is partitioned into interacting subsystems, allowing the region of primary interest to be treated at a high quantum-mechanical level while retaining an efficient and physically consistent description of the environment.[2–5,7] In solvated systems, the external radiation mainly interacts with the solute, while the external medium modifies the response through electrostatic, polarization, and short-range quantum effects.[1,3,4,8] In contrast, metal nanoparticles can absorb the electromagnetic radiation yielding to the collective excitation of localized surface plasmons, which strongly enhance the local field at the surface, and substantially modifying the electronic structure of molecular adsorbates.[6,8] In this contribution, we present an integrated quantum-embedding/classical framework for molecular response properties in complex environments, ranging from solutions to nanostructured materials within a unified formalism.[3–8] The approach is based on multilevel density functional theory (MLDFT), in which the system is partitioned into active and inactive quantum subsystems described at the DFT level, to response theory through coupled-perturbed Kohn-Sham equations for the MLDFT Hamiltonian.[5,7] We showcase the accuracy of the approach for selected systems in solution, and we discuss the challenges for accurately describing hybrid molecule-plasmons systems, especially surface-enhanced spectral response.[4,6,8]

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Acknowledgments:
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Anisotropic plasmonic excitations in quasi-two-dimensional Au(111) slabs

Speaker: Jazmin Aragon Sanchez
Affiliation: University of Rome Tor Vergata

Abstract: We study the optical response of Au(111) slabs from monolayer to few-layer systems using first-principles calculations and a quasi-2D dielectric model. In the long-wavelength limit, a low-energy excitation emerges and strengthens with thickness, signaling collective behavior. The monolayer response is highly anisotropic: an acoustic-like plasmon appears mainly along the Γ–K direction, originating from Coulomb-driven renormalization of interband transitions. Orbital analysis traces this anisotropy to coexisting s and d bands along Γ–K, versus purely s states along Γ–M, consistent with experiments on extended Au(111) surfaces. As layer number increases, directional dependence fades and low-energy modes develop along multiple directions, marking a crossover to bulk-like isotropy. Our results provide a coherent picture of plasmonic excitations across the 2D–3D transition, highlighting the role of orbital texture, interlayer coupling, and momentum-space anisotropy in low-dimensional metallic systems.

Impact of defects on the electronic and transport properties of 2D semiconductors

Speaker: Luca Camilli
Affiliations: University of Rome Tor Vergata

Abstract: Defects are ubiquitous in all materials and have enormous effects on the electronic, magnetic, mechanical and optical properties [1-3]. Using a combination of transport experiments, low-temperature scanning tunnelling microscopy (STM), spectroscopy (STS) and ab initio calculations, we explore the effect of the presence of defects in layered and two-dimensional (2D) semiconductors. We start by discussing how defects and impurities affect the electrical transport in anisotropic 2D materials by investigating the anisotropic layered model system germanium arsenide [4]. In particular, we show that the presence of impurity-induced localized states in the band gap introduces isotropic hopping conduction, which in addition to the intrinsic band conduction significantly influences the anisotropic electrical properties of the material, especially at room temperature, i.e., at application-relevant conditions. Then, we move to ZrSe2 and show that Zr-antisite point defects locally induce a n-type doping which shifts the conduction band minimum below the Fermi level, thereby leading to a semiconductor-to-metal transition and the subsequent formation of a commensurate 2x2 and non-dispersive charge density wave reconstruction [5]. We also discuss line defects such as mirror grain boundaries and edge terminations and find that zigzag- or armchair-terminations exhibit distinct electronic properties. Next, we investigate various types of grain boundaries in chemical vapor deposited MoS2 and observe that some introduce deep in-gap states in the electronic band structure [6]. This information is then used to predict the transport properties of charge carriers across such grain boundaries. Such information is crucial when it comes to performance of devices based on industrially-relevant CVD-grown MoS2. Finally, we report a collection of atomically resolved images of the hyperbolic van der Waals MoOCl2, with a focus on the characterization of the most abundant point defects.

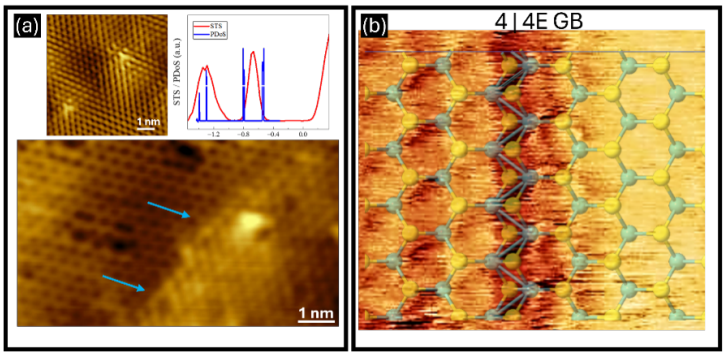

Figure 2: Defects in 2D semiconductors. (a) from top left, clockwise: STM image of two point-defects in mechanically exfoliated ZrSe2; Experimental STS (red curve) and simulated projected density of states (blue lines) of Zr antisite point defect; STM image of a shear-type grain boundary observed in ZrSe2. (b) STM image of 4|4E mirror grain boundary in MoS2, with overlaid its stick-and-ball model

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Optical and Low-Momentum Excitations in 2D Systems from momentum-resolved EELS

Speaker: Alberto Guandalini
Affiliations: University of Rome La Sapienza

Abstract: Momentum-dependent electron energy-loss spectroscopy (q-EELS) has recently proven to be a pivotal tool for investigating charge excitations in suspended low-dimensional (2D) materials using a transmission electron microscope (TEM). With sufficiently high momentum resolution, q-EELS can probe the optical-limit regime ($q \approx 0$) as well as low-momentum dispersions, thus enabling an unprecedented characterization of monolayer materials. In this talk, I will discuss recent advances both in the interpretation of low-momentum measures, along with advances in the calculation of electron-energy losses with many-body perturbation theory, required as electron interaction is enhanced in freestanding 2D materials. Then, I will present recent experimental observations of phonon, exciton, and plasmon dispersions in prototypical 2D materials such as freestanding graphene and monolayer h-BN, and show how their peculiar 2D dispersions can be interpreted with the help of simulations.

Temperature-Dependent nonlinear optics from first-principles: application to Second-Harmonic Generation in few-layers MoS_2

Speaker: Myrta Grüning [1,3], Anna Romani [1,3], Claudio Attaccalite [2,3]
Affiliations: [1] School of Mathematics and Physics, Queen's University Belfast, Belfast, United Kingdom .[2] CNRS/Aix-Marseille Université, Centre Interdisciplinaire de Nanoscience de Marseille UMR, France. [3] European Theoretical Spectroscopy Facilities (ETSF)

Abstract: We present a first-principles real-time approach to study non-linear response of solids at finite temperature. Finite temperature effects are included as the renormalization of the quasiparticle energies and a dephasing term proportional to the quasiparticle lifetimes. We evaluate electron-phonon matrix elements from Density-Functional Perturbation Theory for lattice dynamics and then calculate quasiparticles renormalization and lifetime from the Fan-Migdal and Debye-Waller terms of the electron self-energy. Electron excitations are treated at the independent particle level of approximation. We apply the approach to the second-harmonic generation (SHG) in monolayer and trilayer MoS_2 and compare with existent experiments. A temperature-dependent experiment on those systems showed an enhancement with temperature of the SHG in the monolayer at 900 nm. Our results do not confirm the experimental observation and highlight the need of further experimental measurements and the inclusions in the theory of relevant effects such as thermal expansion.

Polarity-stabilized nonequilibrium excitonic responses in Janus transition-metal dichalcogenides

Speaker: Na Li
Affiliations: Humboldt University of Berlin

Abstract: Two-dimensional transition-metal dichalcogenides exhibit strong excitonic effects, and their optical response can be strongly modified by photoexcited carriers. In this work, we investigate how the built-in out-of-plane polarity of Janus TMDs affects nonequilibrium exciton renormalization. Using real-time TDDFT combined with nonequilibrium Bethe-Salpeter equation calculations, we compare Janus MoSSe with conventional $MoSe_2$ under photoexcited carrier densities from 1.0×10^{12} to 8.3×10^{12} cm^{-2}. Our results show that MoSSe exhibits a much more stable excitonic response than $MoSe_2$. The main exciton peaks in MoSSe remain nearly unchanged, with peak shifts below 30 meV, whereas $MoSe_2$ shows pronounced peak shifts up to about 200 meV together with oscillator-strength redistribution. By separating Pauli-blocking and carrier-induced screening contributions, we find that the strong response of $MoSe_2$ is mainly driven by screening, while both effects are significantly weaker in Janus MoSSe. Further analysis of bright excitons indicates that Janus polarity helps preserve the excitonic structure under photoexcitation. These findings suggest that built-in polarity can suppress carrier-induced exciton renormalization and stabilize nonequilibrium optical responses in two-dimensional Janus materials.

Exciting News

Speaker: Pasquale Pavone
Affiliations: Humboldt-Universität zu Berlin

Abstract: Many modern electronic-structure codes implement methods of theoretical spectroscopy. Among them, exciting is an all-electron full-potential package that has a very rich portfolio of all levels of theory, with a particular focus on excitations. It implements the linearized augmented planewave plus local orbital (LAPW+LO) basis, which is known as the gold standard for solving the Kohn-Sham equations of density-functional theory (DFT). Based on this, it also offers benchmark-quality results for a wide range of excited-state methods. In this talk, I provide a comprehensive overview of the features implemented in exciting in recent years, accompanied by short summaries on the state of the art of the underlying methodologies. They comprise DFT and time-dependent density-functional theory, density-functional perturbation theory for phonons, and electron-phonon coupling, and many-body perturbation theory in terms of the GW approach and the Bethe-Salpeter equation. Moreover, exciting can handle resonant inelastic x-ray scattering, pump-probe spectroscopy as well as exciton-phonon coupling. All aspects are demonstrated with examples for scientifically relevant materials.

Probing Electron-Phonon Interaction with Resonant Inelastic X-ray Scattering

Speaker: M. L. Urquiza [1,2], Davide Sangalli [3,2], and Giovani Onida [1,2]
Affiliations: [1] Physics Department, Università degli Studi di Milano, Italy. [2] European Theoretical Spectroscopy Facility (ETSF). [3] Istituto di Struttura della Materia (ISM—CNR), Area della Ricerca di Roma 1, Italy

Abstract: Resonant inelastic X-ray scattering (RIXS) is a photon-in/photon-out spectroscopic tech- nique that accesses elementary excitations involving various degrees of freedom (spin, charge, lattice, etc.)[1, 2]. Recent progress in synchrotron facilities has made it possible to access phonon excitations with remarkably high resolution, providing momentum de- pendence, element selectivity, and bulk sensitivity. However, interpreting RIXS spectra remains challenging due to the coupling between different excitations. Indeed, although RIXS is used to measure electron–phonon coupling [3], it primarily reveals exciton-phonon coupling, due to the interaction with a core hole [4]. So far, theoretical approaches mainly rely on oversimplified models that use adjustable parameters to fit experimental results, limiting their applicability [5]. The Bethe–Salpeter equation (BSE) represents the state-of-the-art method for describ- ing excitonic effects, as it explicitly accounts for electron–hole correlation, and has been successfully applied to reproduce X-ray absorption and RIXS spectra [6, 7]. Building on this approach, we propose an ab initio method to compute phonon excitations in RIXS by combining the BSE with Density Functional Perturbation Theory (DFPT). In this talk, we will discuss the role of exciton–phonon interactions in RIXS spectra and present preliminary results for hexagonal boron nitride (hBN).

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Resonance Raman scattering with infrared excitation in quantum materials: a joint experimental and Ab-Initio inquiry

Speaker: Leonetta Baldassarre
Affiliations: University of Rome La Sapienza, Italy

Abstract: Resonance Raman scattering provides a valuable probe into the intertwined electronic and vibrational properties of materials by selectively mapping distinct regions of electron and phonon dispersion via tunable laser excitation. I will discuss our experimental approach using a custom-built setup that extends resonance Raman scattering with excitation deep into the near-infrared range. This frequency shift enables the direct investigation of electron-phonon and exciton-phonon interactions, specifically targeting scattering processes resonant with the conduction band minimum of narrow-band layered semiconductors ($MoSe_2$ and $MoTe_2$) and close to the Dirac points of graphene. To isolate the underlying coupling mechanisms, experimental data are systematically compared to ab-initio theoretical calculations. This quantitative experiment-theory comparison permits the unambiguous identification of the phonon modes participating in the resonant processes. Notably, in graphene, this combined approach resolves a momentum-dependent electron-phonon coupling between low-energy carriers and zone-boundary optical phonons. The integration of near-infrared resonance Raman spectroscopy with first-principles theory thus serves as an effective methodology for quantifying the charge-carrier and lattice dynamics that dictate the physics of low-dimensional quantum matter.

Infrared markers of topological phase transitions in quantum spin Hall insulators

Speaker: Paolo Fachin, Francesco Macheda, Paolo Barone, Francesco Mauri
Affiliations: University of Rome La Sapienza

Abstract: Vibrational infrared optical response can be used to discriminate between the electronic topological states of two-dimensional quantum spin Hall insulators (QSHI). First principles phonon infrared spectra of germanene and jacutingaite, Kane-Mele systems of recent experimental investigation, exhibit a large discontinuity concomitant with the topological phase transition [1]. Such significant changes are explained in the framework of the low energy Kane-Mele model by the connection between the vibrational and the electronic responses at the valleys [2]. Even when the infrared active phonon resonate with the energy gap of the material, the vibrational resonances show Fano profiles with remarkable differences in the intensity and the shape between the two topological states [2].

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Ab-Initio pump-probe non-equilibrium exciton dynamics in monolayer hBN

Speaker: Daniel Santos Stone
Affiliations: CNRS/Aix-Marseille University

Abstract: Pump-probe experiments are essential for probing the nonequilibrium optical properties of 2D materials, providing direct, time-resolved access to exciton formation and thermalization dynamics Simulating these dynamics requires a dissipative Bloch equation formalism, such as the recently developed Excitonic Bloch Equations (XBE), which explicitly incorporate exciton-phonon coupling while avoiding Hartree overscreening. Although this theoretical framework exists, a complete, predictive, ab initio computational pipeline for real-time exciton dynamics has yet to be established. A key challenge is the ab initio treatment of exciton-phonon coupling at finite Q itself—a process critical to energy relaxation, spectral broadening, and phonon-assisted luminescence. Computing the necessary exciton-phonon coupling matrix elements presents a major computational obstacle, which must be overcome before reliable dynamical simulations can proceed. Equally central is determining the convergence of different quantities required for the dynamics, such as the different scattering rates, exciton-phonon couplings, exciton dispersions, etc, as these intimately govern the kinetics and interplay of the different exciton species. This presentation will introduce the theory of excitonic pump-probe spectroscopy, detail the theoretical and computational challenges of the XBE, present the first practical numerical convergence thresholds, and showcase different ultrafast real-time pump-probe simulations for monolayer hBN.

The electro-magnetic excitonic displaced Hamiltonian

Speaker: Riccardo Reho [1], Andrea Marini [2]
Affiliation:[1] University of Luxembourg, [2] CNR Istituto di struttura della materia (ISM)

Abstract: We demonstrate, both analytically and numerically, that excitons are not intrinsic excitations of a material but rather emerge as the outcome of the measurement process itself. The excitonic states appear as poles of the response function of an effective Hamiltonian that is displaced from the unperturbed, equilibrium one by an electromagnetic displacement field fixed by the geometry of the external laser [1,2]. Excitons therefore correspond to the linear–response fluctuations of the system about this shifted equilibrium, whereas the intrinsic neutral excitations are the poles of the response functions evaluated at the un–shifted equilibrium. We make this distinction rigorous by showing that, while the equilibrium excitations respect the periodic gauge of the crystal, the excitonic electromagnetic displacement encoded in the exciton definition breaks it. This provides a definitive proof that, in the absence of an external perturbation, the exciton cannot be defined, and clarifies the fundamental role played by the coupling to the Maxwell field in the very notion of an exciton.

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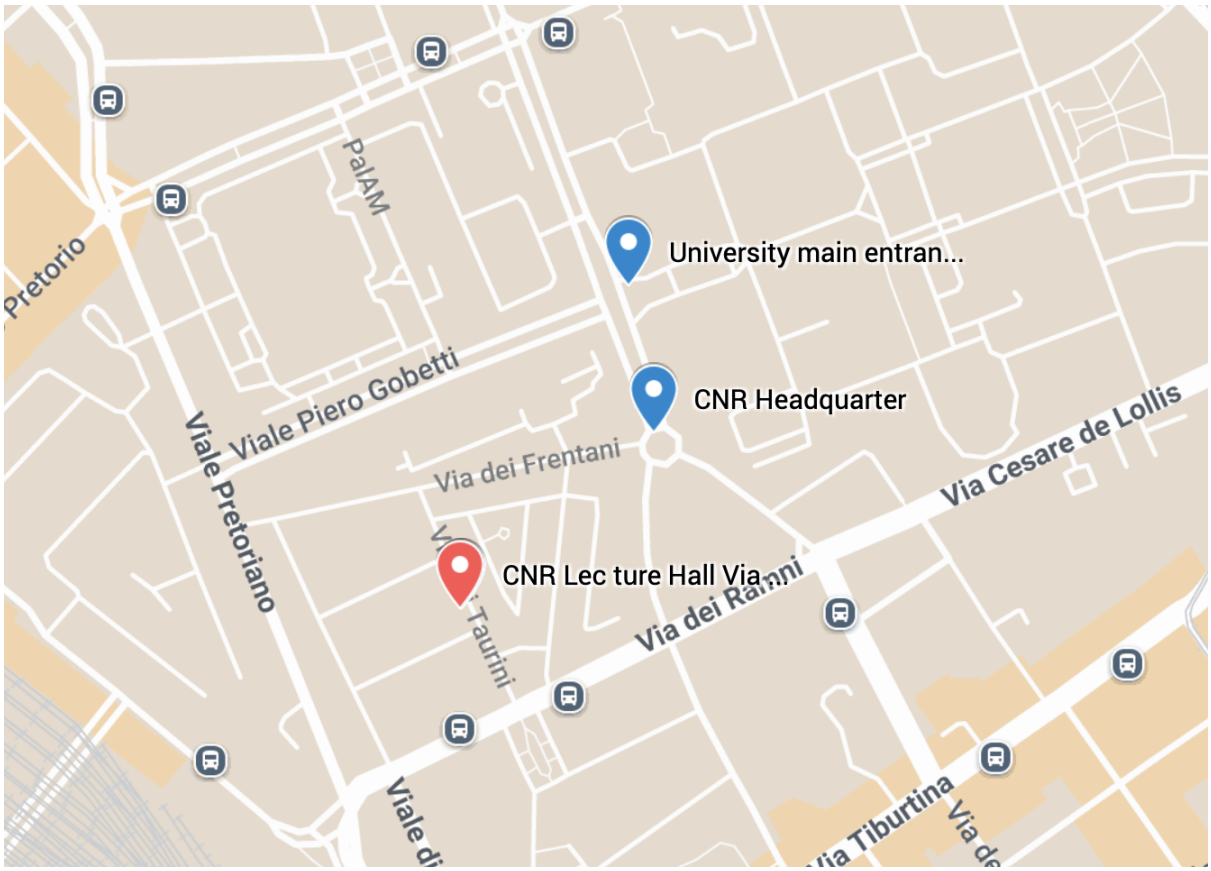
Practical information

4.1. The Venue

The workshop will take place in the CNR Hall located in Via dei Taurini 19. It is located nearby the main entrance of the University La Sapienza and CNR headquarter.



4.2. A Visit to the Fermi Museum

This building was the Royal Institute of Physics of the University of Rome in the late nineteenth century. In the early 1930s, Enrico Fermi and his group — known as "I Ragazzi di Via Panisperna" (Franco Rasetti, Emilio Segrè, Ettore Majorana, Bruno Pontecorvo and others) — conducted here their pioneering experiments on neutron slowing, laying the foundations of nuclear physics and earning Fermi the Nobel Prize in 1938. We will meet at the museum entrance in Piazza del Viminale (the original entrance on Via Panisperna is no longer in use).

The "goldfish fountain", in the courtyard of the Institute where Enrico Fermi, in October 1934, discovered that water could slow neutrons and make them far more effective at triggering nuclear reactions, a finding central to his 1938 Nobel Prize in Physics.

Acknowledgements

This workshop has also been funded by the local **CECAM-IT-SIMUL** node of the Centre Européen de Calcul Atomique et Moléculaire (CECAM), represented at Council by the Istituto Italiano di Tecnologia (IIT). The node is sponsored by a Consortium of Italian Institutions comprising the Polytechnic University of Milan, the Polytechnic University of Turin, the University of Rome Tor Vergata, the University of L'Aquila, Sapienza University of Rome, the Istituto Italiano di Tecnologia (IIT), the University of Calabria, the University of Pavia, the University of Bologna and Cineca, the University of Naples Federico II, and the University of Cagliari.

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