Quantum Espresso

Applications for Material Sciences and Chemistry

Book of Abstracts



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Opening Talk

Polarons in 2D materials and in halide perovskites using the EPW code

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The aim of this talk is twofold: First, to introduce the EPW code, a core module of the Quantum ESPRESSO materials simulation suite which specializes on high-accuracy calculations of electron-phonon interactions and related materials properties; Second, to describe some recent applications of EPW to the study of polarons in two-dimensional crystals and halide perovskites.

Since its creation in 2006, the EPW code has grown to become a fully-fledged tool for advanced many-body calculations of electron-phonon physics, including carrier transport and magnetotransport, superconductivity, phonon-assisted optics, polarons, and thermal band structure renormalization. Here, I will briefly introduce the EPW development team, review the structure and capabilities of EPW, and discuss ongoing developments and future directions.

As an example application of EPW, I will describe recent work on polarons. The polaron is an emergent quasiparticle consisting of an electron dressed by a cloud of virtual phonons, and is responsible for a plethora of unconventional transport and optical properties. Recent experimental investigations highlighted the importance of polarons in interesting classes of materials such as boron nitride, transition metal dichalcogenides, and halide perovskites. Here, I will discuss the structure and energetics of polarons in representative systems of these classes. In particular, I will show how phonon-induced electron localization leads to a rich variety of quasiparticles of all sizes and shapes, and raises interesting questions on our current understanding of electron dynamics in complex materials.

Day 1 - Session 1

Efficient many-body perturbation theory calculations in 2D materials: Applications to ARPES and EELS of Graphene (IT)

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Many-body perturbation theory methods are able to accurately predict quasiparticle (QP) and spectroscopic properties of several classes of materials. However, the calculation of the QP band structure of 2D materials is known to require a very dense BZ sampling. For 2D semiconductors, large **q**-point grids are required to describe the sharp **q**-dependence of the dielectric matrix in the long-wavelength limit ($\mathbf{q} \rightarrow 0$).

In this talk, I will first describe a new methodology able to drastically improve the convergence of the QP corrections in 2D semiconductors with respect to the BZ sampling by combining a Monte Carlo integration method with an interpolation scheme able to describe the sharp dispersion of the dielectric function. Then, I will show how to integrate the new methodology with a multi-pole expansion of the frequency dependence of the screening, able to reach the accuracy of full-frequency methods with a coarse sampling of the frequency space. The combined approach will be used to obtain accurate results for graphene QP band structure. The latter is finally used to calculate electron energy loss spectra (EELS) of graphene at finite momentum transfer via the Bethe-Salpeter equation (BSE), showing excellent agreement with recent high-resolution experimental data, provided that the electron-hole interaction is properly taken into account.

Impressive electronic and thermal transports in CsK₂Sb: A thermoelectric perspective (CT)

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Over the past 2 decades, there has been active research into the hunt for innovative thermoelectric materials with a high value of the figure of merit. To investigate the potential of CsK₂Sb as a thermoelectric material, we analyzed its electrical and thermal transport properties using density functional theory and Boltzmann transport theory. We found that CsK₂Sb is a direct band gap material with a band gap of 1.44 eV using the Gaussian-attenuating Perdew–Burke–Ernzerhof functional with spin–orbit coupling. Using electron–phonon Wannier calculations, we computed the electron–phonon lifetimes for electrons and holes, which are leveraged to estimate absolute values of the electronic transport coefficients by solving the Boltzmann transport equation for electrons. At 300 K, we have found that CsK₂Sb exhibits a maximum value of power factor of 5.7 mW K⁻² m⁻¹ with electron doping, which is comparable to those of well-known thermoelectric materials. By solving the Boltzmann transport equation for phonons, we demonstrate that CsK₂Sb has significantly lower phonon group velocity and phonon–phonon lifetimes than other well-known thermoelectric materials, resulting in an ultralow lattice thermal conductivity of 0.25 W m⁻¹ K⁻¹ at 300 K. At 500 K, CsK₂Sb showcases an exceptional figure of merit of 4.69 (2.48) with electron (hole) doping, surpassing all other full Heusler alloys. These findings reveal that CsK₂Sb is a "phonon glass electron crystal", a property of an ideal thermoelectric material.

Using QE for evaluating nanomaterials as neural nanostimulators with a focus on magnetoelectric nanoparticles (CT)

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In the pursuit of advanced brain-machine interfaces, the development of non-invasive techniques for stimulating neurons has garnered substantial interest. One form of such a neural stimulator is magnetoelectric nanoparticles (MENPs). A MENP made up of two-phase, spherical structure of cobalt ferrite (core) and barium titanate (shell) can convert an input magnetic field to an output electric polarization which can be utilized to selectively stimulate neurons. This energy conversion relies on the property of magnetostriction exhibited by cobalt ferrite and piezoelectricity of barium titanate. These properties are in turn a function of other material properties such as elastic constants, magnetostriction, piezoelectricity etc. of the constituent phases. Therefore, in order to quantify the magnetic to electric energy i.e. the magnetoelectric co-efficient of a MENP, it is important to determine these material properties. However, classical experimental methods often fall short when investigating these materials at the nanoscale as they are generally tailored to bulk properties or their exists difficulties in preparing nanoscale samples.

To address this challenge, we employed Density Functional Theory (DFT) simulations using Quantum Espresso to probe the fundamental characteristics of ME nanoparticles, in particular the elastic constants of the individual phases, which are crucial for understanding the mechanical behaviour of nanoparticles and the evaluation of piezoelectric constants for barium titanate. The knowledge gained through these computational insights and supplemented by experimentally obtainable nanoscale parameters allowed us to inform a Finite Element Analysis (FEA) Model for the simulation of a MENP under an applied magnetic field. To validate our findings, we evaluated the stimulation from the generated electric polarization of the MENPS against in-vivo experimental data.

We used this methodology of combining DFT calculated properties with finite element analysis to study two other types of nanoscale neural stimulators: magnetomechanical ion channel opening (Gregurec, D., et al., ACS Nano, 2020), and piezoelectric electrical stimulation (Ciofani, G., et al., ACS Nano, 2010), using magnetic and ultrasound input carrier signals, respectively.

We envision our method as a foundation for the straightforward evaluation in the field of novel neural stimulation technologies, thus fostering the advancement of nanoscale devices and their potential applications in brain-machine interfaces.

References

- D. Gregurec, A. W. Senko, A. Chuvilin, P. D. Reddy, A. Sankararaman, D. Rosenfeld, P.-H. Chiang, F. Garcia, I. Tafel, G. Varnavides, E. Ciocan, & P. Anikeeva, "Magnetic Vortex Nanodiscs Enable Remote Magnetomechanical Neural Stimulation", ACS Nano 14, 8036-8045 (2020)
- G. Coifai, S. Danti, D. D'Alessandro, . Ricotti, S. Moscato, G. Bertoni, A. Falqui, S. Berrettini, M. Petrini, V. Mattoli, & A. Menciassi, "Enhancement of Neurite Outgrowth in Neuronal-Like Cells following Boron Nitride Nanotube-Mediated Stimulation", ACS Nano 4, 6267-6277 (2010)

Pushing the frontiers of Hubbard functionals: First-principles U and V in Quantum ESPRESSO (IT)

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Density-functional theory (DFT) with extended Hubbard functionals is a powerful method for studying complex materials containing transition-metal and rare-earth elements, owing to its accuracy in correcting selfinteractions and its low computational costs [1]. Recently, we developed an automated and reliable approach for the first-principles determination of the on-site U and inter-site V Hubbard parameters using density-functional perturbation theory (DFPT) [2-4]. In this talk I will show that DFPT allows us to reduce significantly computational costs, improve numerical accuracy, and fully automate the calculation of the Hubbard parameters by recasting the linear response of a localized perturbation in supercells into an array of monochromatic perturbations that can be calculated in the primitive cell. This framework can be used with different Hubbard manifolds, such as nonorthogonalized and orthogonalized atomic orbitals, including the respective calculation of Pulay (Hubbard) forces and stresses [5] that are needed for the self-consistent evaluation of Hubbard parameters [3]. I will show how this formalism can be used for the calculation of such properties as voltages in Li-ion batteries [6,7], formation energies of oxygen vacancies in perovskites [8], and I will discuss the applicability of this formalism for improving band gaps with respect to standard DFT [9] and its use for searching of novel materials for the photocatalytic water splitting [10]. Finally, I will present the extension of this framework to the calculations of phonons [11] and electron-phonon coupling [12] in selected transition-metal compounds. These tools are implemented in the open-source Quantum ESPRESSO distribution [13] and are available to the community at large.

References:

- 1. V. L. Campo Jr and M. Cococcioni, J. Phys.: Condens. Matter. 22, 055602 (2010)
- 2. I. Timrov, N. Marzari, M. Cococcioni, Phys. Rev. B 98, 085127 (2018)
- 3. I. Timrov, N. Marzari, M. Cococcioni, Phys. Rev. B 103, 045141 (2021)
- 4. I. Timrov, N. Marzari, M. Cococcioni, Comput. Phys. Commun. 279, 108455 (2022)
- 5. I. Timrov, F. Aquilante, L. Binci, M. Cococcioni, N. Marzari, Phys. Rev. B 102, 235159 (2020)
- 6. I. Timrov, F. Aquilante, M. Cococcioni, N. Marzari, PRX Energy 1, 033003 (2022)
- 7. I. Timrov, M. Kotiuga, N. Marzari, Phys. Chem. Chem. Phys. 25, 9061. (2023)
- 8. C. Ricca, I. Timrov, M. Cococcioni, N. Marzari, U. Aschauer, Phys. Rev. Research 2, 023313 (2020)
- 9. N.E. Kirchner-Hall, W. Zhao, Y. Xiong, I. Timrov, I. Dabo, Appl, Sci. 11, 2395 (2021)
- 10. Y. Xiong et al., Energy Environ. Sci. 14, 2335 (2021)
- 11. A. Floris, I. Timrov, B. Himmetoglu, N. Marzari, S. de Gironcoli, M. Cococcioni, Phys. Rev. B 101, 064305 (2020)
- 12. J.-J. Zhou, J. Park, I. Timrov, A. Floris, M. Cococcioni, N. Marzari, M. Bernardi, Phys. Rev. Lett. 127, 126404 (2021)
- 13. P. Giannozzi et al., J. Phys.: Condens. Matter 29, 465901 (2017)

Day 1 - Session 2

Optical signals of qubits in defected 2D TMDs (IT)

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It has been shown that intrinsic properties alone cannot sustain long lived spin signals in transition metal dichalcogenides (TMDs) and that these must come from extrinsic properties [1]. Here defects play a crucial role by enriching the optical properties of a material. In this work we link different types of defects to specific optical signatures by employing many-body perturbation theory with the Yambo package to obtain the optical absorption spectra of defected TMDs.

We find that the largely unstudied metal vacancies show a larger set of polarized excitons than chalcogen vacancies, introducing localized excitons in the sub-optical-gap region [2] whose wave functions and spectra make them good candidates as quantum emitters. However, when dealing with substitutional defects, the spin texture and pristine exciton energies are preserved, despite the strong interaction with the defect. Still, as the full optical-gap region remains free, these defects can be used as sites for grafting and patterning in optical detectors. A redistribution of excitonic weight between the A and B excitons is visible in both cases and may allow the quantification of the defect concentration. This work establishes excitonic signatures to characterize defects in 2D materials and highlights vacancies as qubit candidates for quantum computing.

References

- 1. M. Ersfeld, F. Volmer, P. Melo, et al, Nano Lett. 19, 4083 (2019)
- 2. P. Melo, Z. Zanolli, M. Verstraete, Adv. Quantum Technol. 4: 2000118 (2021)

Electronic properties and defect levels induced by n/p-type defect-complexes in Ge (CT)

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Defect-complexes are point defects that significantly influence the geometric, optical, and electrical properties of materials. The presence of defect-complexes in Ge have been reported to be electrically active and influence the performance of its device. Despite of this breakthrough, several defect-complexes in Ge are not well understood; hence may pose as a challenge to the optimal performance of Ge based devices. In this study, hybrid density functional theory calculations of substitution and interstitial defect-complexes in Ge were performed. Their formation energies, electronic properties, defect-complex stability and induced defect levels were predicted. While the formation energies of the defect-complexes formed by the P and Al atoms were relatively low and energetically more favourable, those defect-complexes significantly bound with energies lower than their formation energies. The BGeNi and NGeBi behaved as p-type semiconductors, whereas the SbGeIni, AsGeGai, and PGeAli exhibited n-type semiconductor characteristics. The NGeBi, AlGePi and PGeAli essential donor levels were in the band gap of Ge. A shallow double acceptor level was found to be associated with the AlGePi, while the InGeSbi induced a shallow double donor defect level. The results of this report are important, as they provide insight for the control of n/p-type substitution and interstitial defect-complexes in Ge during synthesis and characterization.

Electronic structure, optical and thermal properties of SrTiO₃ perovskite – A DFT+U study (CT)

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The structural, electronic, optical, elastic, and ferroelectric characteristics of cubic strontium titanate (SrTiO₃) with the space group $(Pm\bar{3}m)$, have been computationally assessed through density functional theory (DFT). In this analysis, the Projector Augmented Wave (PAW) pseudo-potential was employed in conjunction with the Perdew Burke Ernzerhof (PBE) exchange-correlation functional within the framework of the Generalized Gradient Approximation (GGA). Two distinct scenarios were considered: one with and one without the incorporation of the Hubbard U potential [U(Ti_{3d} & O_{2p}) = 5 eV]. These calculations were carried out using the **Quantum** Espresso computational tool. One of the key aspects under investigation was the band gap of cubic $SrTiO_3$ (STO), which was determined by analyzing the electronic band structure at the Gamma point. The results revealed a band gap value of 2.2135 eV when utilizing the standard DFT method and 3.7625 eV when applying the DFT+U approach. Notably, the DFT+U method demonstrated a closer alignment with experimental data. In the context of DFT+U, the PDOS shifts arise from the on-site electron interaction correction. It was observed that the Ti_{3d} and O_{2p} orbitals exhibited a robust hybridization, signifying a covalent bond, substantiated by the overlapping charge density evident in the 2D contour map, Conversely, an ionic bond prevailed between strontium (Sr) and oxygen (O) atoms. Both DFT and DFT+U methods are employed to compute complex dielectric function components, and optical parameters such as reflectivity, refractive index, extinction coefficient, absorption coefficient, and the electron energy-loss spectrum. It was elucidated that the inclusion of the Hubbard U potential played a pivotal role in density functional theory calculations, resulting in a narrower and more experimentally congruent optical spectrum, a significant contrast to standard DFT calculations, which lack this corrective measure and consequently generate broader and less precise electronic bands and optical spectra, particularly in cases where strong electron-electron interactions prevail. Thermal properties like entropy and heat capacity are typically less sensitive to on-site electron correlations, which Hubbard U in DFT+U addresses. Therefore, both standard DFT and DFT+U yield similar results for these properties as electron correlations have a relatively minor impact in this context and have good agreement with the Debye model. Elastic properties, including the Bulk Modulus, Young's Modulus, Shear Modulus, and Poisson's Ratio, were assessed via both cases, yielding closely aligned values, indicative of their consistency and agreement.

Quantum Espresso : Applications for Material Sciences and Chemistry

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Day 2 - Session 1

Non-covalent interactions and chemical bonding in Quantum ESPRESSO (IT)

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Quantum ESPRESSO (QE) is one of the leading software suites for materials modeling, implementing densityfunctional theory (DFT) in the plane-waves/pseudopotentials and projector augmented wave (PAW) approaches. Non-covalent interactions are important in materials that are weakly bound, such as molecular crystals or twodimensional layered van der Waals solids. To describe these interactions accurately, a dispersion functional is required that augments that incorporates van der Waals interactions into the base density functional method. This talk is divided in two parts. First, we will talk about the exchange-hole dipole moment (XDM) model of dispersion and its implementation in Quantum ESPRESSO. XDM is easy to use and one of the most accurate dispersion corrections available, excellent for any system where non-covalent interactions dominate binding. Second, we will explore the use of the companion program critic2 [1,2] to extract chemical information from the converged QE density and wavefunction. In particular, we will see how to extract and plot the electron density and related quantities, find and calculate properties and critical points and compute delocalization indices in solids using maximally localized Wannier functions.

References

- 1. https://github.com/aoterodelaroza/critic2
- 2. https://aoterodelaroza.github.io/critic2

Electron Spin Resonance studies from first-principles: the case of boron in silicon carbide (CT)

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Despite advances toward improving the quality of p-type 4H-SiC substrates and layers, until recently we were still missing a model capable of accounting for the multitude of boron-related optical, junction, and paramagnetic resonance experiments available in the literature. A conspicuous puzzle was the observation of two shallow boron defects with rather distinct axial orientations as found by Electron Spin Resonance (ESR) and Electron Nuclear Double Resonance (ENDOR) data. This feature is not observed in material doped with other group-III elements. Another open issue involved conflicting conclusions from photoluminescence and ESR studies of a deeper boron center, which had been linked to rather distinct models, either based on substitutional or vacancy-related boron defects. We will describe how these problems were recent unlocked by first-principles studies [1], which included the calculation of the electronic activity and the use of the ESPRESSO/GIPAW codes for the evaluation of paramagnetic response of boron defects in 4H-SiC.

References

1. V. J. B. Torres, I. Capan, and J. Coutinho, Physical Review B 106, 224112 (2022)

Why yttrium hexaboride exhibits a much higher superconducting critical temperature than near-identical lanthanum hexaboride: a chemical bonding study under phonons (CT)

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Though YB₆ and LaB₆ share the same crystal structure, atomic valence electron configuration, and phonon modes, they exhibit drastically different phonon-mediated superconductivity. YB₆ superconducts below 8.4 K, giving it the second-highest critical temperature of known borides. LaB₆ does not superconduct until near-absolute zero temperatures, however. Though previous studies have quantified the canonical superconductivity descriptors of YB₆'s greater Fermi-level (E_F) density of states and higher electron-phonon coupling (EPC), the root of this difference has not been assessed with full detail of the electronic structure. Through chemical bonding, we determine low-lying, unoccupied 4f atomic orbitals in lanthanum to be the key difference between these superconductors. These orbitals, which are not accessible in YB₆, hybridize with π B-B bonds and bring this π -system lower in energy than the sigma B-B bonds otherwise at E_F . This inversion of bands is crucial: the phonon modes we show responsible for superconductivity cause the sigma-orbitals of YB₆ to change drastically in overlap, but couple weakly to the π -orbitals of LaB₆. These phonons in YB₆ even access an electronic-state crossing, indicating strong EPC. No such crossing in LaB₆ is observed. Finally, a supercell (the *M* k-point) is shown to undergo a Peierls-like effect in YB₆, introducing additional EPC. Use of Quantum Espresso's EPC functionality for determination of the relevant modes and supercells, coupled to the electronic structure of these two borides, is discussed.

Strongly anharmonic lattice vibrations and superconductivity (IT)

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In this talk I will discuss that often the standard treatment of lattice dynamics in the harmonic approximation breaks down and a non-perturbative treatment of anharmonicity is needed to describe the ionic fluctuations of the system. This occurs for instance in systems close to second-order displacive phase transitions, like ferroelectric or charge-density wave transitions, or in materials with large electron-phonon coupling and light atoms, like superconducting hydrides. I will show how the stochastic self-consistent harmonic approximation (SSCHA) method can be used for dealing effectively with this situation. I will describe as well some applications to have high- T_c hydrides like LaH₁₀.

Day 2 - Session 2

Water splitting on transition metal oxide surfaces: insights from DFT (IT)

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In this presentation I will show how DFT calculations can help to better understand the performance of a material as a catalyst for the water splitting reaction.

In order split water molecules into oxygen and hydrogen, two distinct half-reactions need to be catalyzed: the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). I will argue that the OER is by far more difficult to catalyze efficiently, and for the case of iron oxide (Fe₂O₃, hematite), I will explain which insights can be gained from DFT. I will also talk about the limits of the standard approaches to this problem, and discuss possible future avenues to improve upon those.

Synergistically driven CoCr-LDH@VNiS $_2$ as a electrocatalyst for overall water splitting (CT)

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Harnessing alternatives to fossil fuels persists to be a major problem for civilization. In this situation, effective earth-abundant water splitting catalysts are necessary to achieve a sustainable future. Here, using density functional theory (DFT) and a number of active sites on the surface selected to adsorb the H, OH, and OOH, we studied the effects of the electronic structures of VNiS₂ and CoCr-LDH on both HER and OER at the atomic level. The various characteristics of pristine LDH (CoCr) and TMDC (VNiS₂) have been investigated within the framework of DFT as applied in the Quantum Espresso Package. As theoretical simulations have proven to be effective in reveling the links between the electronic structure of materials and their catalytic activity. To study the performance towards HER, the hydrogen adsorption on various sites (Ni, V, and S) is examined, in VNiS₂ and CoCr-LDH (Cr-top, Co-top, and hollow). For OER, the Co sites in CoCr-LDH and S sites in VNiS₂ were chosen for mechanism and calculations. The analysis of HER and OER (Adsorption energy, Gibbs Free Energy, and TDOS) makes it abundantly evident that VNiS₂ incredibly increase the catalytic activity in comparison to CoCr LDH. When it comes to OER activity, CoCr LDH outperform VNiS₂. The results offer a fresh method for the logical design and amalgamation of top-notch catalysts for overarching water splitting.

New wide bandgap semiconductor pentagonal cpn monolayer: Ab initio investigation (CT)

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Pentagonal two-dimensional ternary monolayer represent a promising category of materials with distinctive features and a wide array of potential applications. In our work, we have utilized first-principles density functional theory (DFT) calculations using quantum espresso code to identify a novel pentagonal structure, denoted as p-CPN. This newly discovered p-CPN exhibits robust geometric, thermodynamic and mechanical stability, making it a compelling candidate for experimental exploration. Furthermore, this p-CPN demonstrates an indirect bandgap semiconductor behavior, which can be readily tuned by applying equi-biaxial strain. Its mechanical strain tolerance. Moreover, the p-CPN show a notable anisotropic optical response characterized by strong absorption of ultraviolet (UV) light, low reflectivity, and small electron energy loss, making it a promising material for applications in optoelectronics and nanomechanics.

Strain engineering in 2D materials: from first principles to experimental realization (IT)

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The application of strain in 2D materials serves as a powerful tool, not only for the precise tailoring of material properties to meet specific application demands and driving the development of cutting-edge technologies but also for the advancement of our comprehension of fundamental scientific principles. It unveils the complex interplay and interdependence between material structures and physical properties, often shedding light on the intricate, underlying mechanisms that govern their behavior.

During this presentation, I will provide a series of illustrative examples where we employ Density Functional Theory (DFT) calculations, using Quantum Espresso, to understand the impact of strain in 2D materials. Through these examples, we will uncover the subtleties and intricacies of how strain influences these materials at a fundamental level. Following this exploration, we will engage in a thoughtful discussion of the practical implications of these theoretical insights, highlighting their relevance and potential impact on experimental implementation, thereby bridging the theoretical and practical aspects of strain engineering in 2D materials.