



Many-Body Perturbation Theory and Excited-State Simulations

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BOOK OF ABSTRACTS

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[P01] Pressure And Magnetic Field Control Of The Topological Phase In Antiferromagnetic Bilayers

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Antiferromagnetic bilayers are said to be A-type when spins align ferromagnetically within each layer but point in opposite directions in the two layers, resulting in a zero net magnetization. The opposite orientation of majority spins in the two layers strongly suppresses interlayer hopping and the electronic structure is not affected significantly by a change in interlayer distance. Nonetheless, an external magnetic field can drive a metamagnetic transition into a fully ferromagnetic state, where spins in both layers are parallel, so that interlayer hopping is possible and energy bands are sensitive to the separation between the layers. This difference can be exploited to manipulate the energy bands of an A-type antiferromagnetic bilayer by means of the combined effect of pressure and magnetic field. Here we consider bilayer CrSBr as a prototypical example and show using first-principles simulations that pressure affects the interlayer distance, enhancing the interlayer hopping in the ferromagnetic state, and eventually closes the energy gap, inducing a topological phase transition. Remarkably, depending on the magnetization direction it is possible to tune the system either in a quantum anomalous Hall insulating state when spins are out-of-plane or into a half Chern-Weyl semimetallic phase when spins are in-plane, with the emergence in both cases of topological edge states. We expect this phenomenon to be general to A-type antiferromagnetic bilayers, opening interesting perspectives on the manipulation of their topological character towards applications in spintronics and quantum computation.

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[P02] Exploring Reaction Pathways in Molecules and Solids with the NEB Method in CRYSTAL

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Understanding how atoms rearrange during chemical reactions is essential to model reactivity in both molecules and materials. We have implemented the Nudged Elastic Band (NEB) method in the quantum chemistry code CRYSTAL, allowing efficient calculations of reaction mechanisms and energy barriers using localized Gaussian basis sets. The method has been tested on a variety of systems: from simple gas-phase reactions such as hydrogen abstraction, to surface processes such as formamide formation on water ice under astrochemical conditions and solid-state proton jump in a zeolite. Our implementation handles both molecular and periodic systems, allows full optimization of atomic positions for molecules and fixed-cell NEB for solids, and supports advanced features such as image climbing for the detection of transition states. In the future, we aim to extend this tool with generalized solid state NEB and variable-cell methods, as well as parallelization to accelerate convergence for large-scale systems.

[P03] Modelling Optical Properties of Nickel Iodide with many-body effects.

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The prediction of polarization and optical responses is essential for understanding charge transfer properties and identifying functional materials for defect engineering, with the ultimate goal of developing optimal systems for single-photon emitters.

To this end, the Nickel lodide magnetic cell is simplified to capture the antiferromagnetic behavior arising from the helicoidal, incommensurate magnetic periodicity within the layers, where the direction of magnetization alternates between adjacent layers. Various magnetic unit cells are explored to identify the one that best reproduces the observed experimental features.

Using DFT (and DFT+U), we obtain the optimized basis set for the ground state. To go beyond linear response theory, we employ the Yambo ab initio approach, which allows for the description quantitative of optical properties in systems—such out-of-equilibrium involved as those in pump-probe experiments-by real-time integration of the Schrödinger equation. The desired level of approximation is by incorporating many-body effects achieved through many-body perturbation theory.

[P04] Implementation of Functional Derivatives for GGA Functionals in Yambo code

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Density Functional Theory (DFT) is a widely-used computational approach for investigating electronic properties of materials, relying heavily on the choice of appropriate exchange-correlation functionals. Among these functionals, the generalized gradient approximation (GGA) is widely used because it considers not only electron density but also its gradient (variation) to better describe electron interactions beyond simpler approximations. In this poster, we present two implementations for calculating exchange-correlation kernel tensor; one using libxc, and one numerical. Numerical stability for some 2D and 3D systems is assessed. Results are validated by spectra obtained from real-time propagation of density matrix.

[P05] Tuning the electronic properties and spin-textures in buckled two-dimensional compounds

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Two-dimensional buckled materials caught the attention in electronics and spintronics due to their peculiar properties, such as the ferroelectricity, and high tunability. The latter means that their properties strongly depend on some parameters such as the number of layers, the way in which they are stacked on top of each other, the presence of external fields or pressures.

Through ab initio simulations, we can construct a virtual laboratory, when we can manipulate such parameters and investigate their influence on the behaviour of the compounds under consideration.

We did this kind of analysis for some binary compounds of the MX type, where M and X belongs either to III and V (GaAs, GaP) or both to the IV (GeSn) group of the periodic table, in their two-dimensional form. We investigated the structural, electronic and spin-related properties of such layered materials in different configurations, identifying the most stable ones and focusing on the differences between the various systems.

In doing this, it is necessary to deal with the functionality and limitations of the software used, in this case the Quantum Espresso package. For example, for the materials here analyzed, it is necessary to employ the supercell method to prevent periodic replicas from interacting with each other, and the dipole correction to cure the spurious dipole moment induced by periodic boundary conditions. Furthermore, a proper account of the interlayer van der Waals interaction is of utmost importance, that in our calculations is introduced to suitable non-local van der Waals functionals.

[P06] Fast Inertial Relaxation Engine as structural optimization method in CRYSTAL code

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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-Goldfarb-Shanno (BFGS) formula. At the same time, recent works have highlighted that the so-called Fast Inertial Relaxation Engine (FIRE), an optimization method 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 mechanical package for condensed quantum matter simulations. The efficiency of FIRE algorithm has been for different atomic with assessed systems 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 (NEB) method.

[P07] Electronic Excitations and Photoisomerization Dynamics in Photoswitch–Quantum Dot Nanohybrids: A Correlated Approach

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The integration of molecular photoswitches (PhSs) with semiconductor quantum dots (QDs) into hybrid nanosystems (PhS+QD) enables tunable optoelectronic behavior, with applications in biomedicine, catalysis, and sensing [1]. However, accurately describing their electronic structure and photoisomerization dynamics remains challenging. As QD size increases, computational complexity grows rapidly, making it difficult to fine-tune exciton energy resonance between the two components [2]. Standard computational approaches often neglect key many-body interactions, failing to capture crucial photochemical features such as conical intersections and avoided crossings [3].

To address this, we apply Hybrid Configuration Interaction (HyCI), a methodology that combines electronic structure techniques—such as (Full) Configuration Interaction and (Time-Dependent) Density Functional Ty—to accurately describe electronic excitations in PhS+QD systems. The angular momentum selection rules for the QD, along with the effective mass and envelope function approximations, make calculations computationally feasible while incorporating essential correlation effects.

Using HvCl, we investigate a functionalized azobenzene coupled with a cadmium selenide QD, providing a detailed description of the hybrid potential energy surface, dipole moments, and absorption spectra along the primary photoisomerization coordinate. Our results reveal two asymmetric avoided crossings at resonance, which may significantly influence the efficiency of photoisomerization during the picosecond-scale exciton lifetime. These findings highlight the critical role of many-body effects in PhS+QD nanohybrids and underscore the necessity of correlated methodologies for accurately describing their dynamics. photoisomerization Future work will explore quantum yields and reaction pathways using nonadiabatic quantum molecular dynamics simulations.

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[P08] Optical Properties of Cementitious Oxides for Design of Photonic Metaconcrete – an Ab initio study

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Concrete is the single most commonly produced material by humans. As a consequence, buildings account for approximately 40% of total electricity consumption. There is therefore an urgent need to reduce the environmental impact of concrete throughout its lifecycle. A solution we propose is to reduce the energy consumption of buildings by exploiting the radiative cooling phenomenon [1]. In this sense, the MIRACLE (Photonic Metaconcrete with Infrared RAdiative Cooling capacity for Large Energy savings) project is pioneering a new generation of green concrete capable of

passive cooling [2]. The radiative cooler dissipates heat within the atmospheric transparency window (ATW), a range of infrared frequencies to which the atmosphere is permeable. The heat emitted within the ATW escapes the atmosphere and dissipates into space. This allows the object to thermally couple to an environment that is significantly colder than its surroundings and effectively cool down. In practice, the research aims to develop photonic concrete by employing structured metamaterials [3] to manipulate the absorption and emission spectrum of concrete. To engineer effective daytime radiative coolers, we need to find materials whose emissivity

matches the ATW. Additionally, to minimize heat absorption from the sun, the metaconcrete has to exhibit high reflectivity at frequencies outside the ATW range. Both absorbance and reflectance are inherent material characteristics linked to their optical dielectric properties, which originate at the atomic and electronic level and can be accurately predicted by first principles calculations. To advance the ideas of photonic concrete, we provide an overview of the optical properties and excitonic spectra of relevant cement and concrete phases. We calculate the frequency-dependent dielectric function using various levels of approximation [4]. namely the GW approximation [5] and the Bethe-Salpeter equation (BSE) [6]. Our particular focus is on understanding the excitonic properties of basic oxides such as CaO, SiO2, Al2O3 and Fe2O3 which serve as building blocks for complex cement oxides like alite (Ca3SiO5) and belite (Ca2SiO4). Additionally, we investigate other clinker phases, including gypsum (CaSO4.2H2O) and calcium sulfate (CaSO4), as well as hydrated phases like portlandite (Ca(OH)2) and tobermorite (Ca5Si6O16(OH)2.4H2O/ Ca5Si6O16(OH)2.7H2O), among others.

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[P09] Ab-initio Study of ZrO2 Polymorphs: Optical Properties Including Excitonic Effects

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Accumulation of hydrogen is a prior security issue that can endanger the nuclear facilities integrity. Radiolysis of water is a phenomenon of special relevance in the nuclear industry and management of nuclear waste, given that free radicals production leads to materials corrosion and release of hydrogen gas. The thin-walled metal tube that wraps nuclear fuel rods, known as cladding, is preferentially made of zirconium-based alloys. Fundamental to corrosion resistance is the build up of a passive and protecting dense oxide layer (ZrO2, zirconia) in water exposed alloy surfaces. A thorough study of Petriket al., where a number of oxides were subjected to y radiation, showed that oxides with a band gap around 5 eV evinced increased adsorbed water dissociation rates, this is the case of ZrO2 [1]. The authors explain their observation in terms of a resonant energy transfer mechanism between an exciton guasiparticle created in the bulk of the oxide that migrates towards its surface. The band gap of the oxide has to be similar to, larger than indeed, the O-H bond breaking energy. Description of optical properties is shown to pose a great challenge for single-particle formalisms based on Fermi's Golden Rule. Conversely, an accurate reproduction of experimental data is achieved with many-body perturbation theory methods built on Green's functions within the GW approximation to solve the Bethe-Salpeter equation (BSE)

to model excitonic quasiparticles features in the absorption spectrum. In this contribution, we report the electronic band structure calculated at the quasiparticle level of approximation and the optical absorption spectra of the cubic phase of ZrO2, including full excitonic features in the modelling.

[P10] Photoemission Tomography for Excitons in Periodic Systems

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The momentum space signatures of quantum mechanical states and their removal energies can be experimentally accessed by means of angular-resolved photoelectron spectroscopy (ARPES). For the ground state and by treating the photoelectrons as plane waves, photoemission (orbital) tomography (POT) establishes a particularly simple connection of the momentum space signatures and the quantum mechanical wave functions in real space via a Fourier transform relation. Here, we extend the POT technique to the case of photoemission from excitons, which then allows for direct comparison to experimental data in time-resolved (pump-probe) ARPES experiments. Our approach has been tested for isolated molecules in the gas phase on a real-space grid, and was recently extended to periodic systems treated in a plane wave basis set. It can be combined with excitons either obtained from Casida calculations or within the framework of the Bethe-Salpeter equation.

[P11] Probing and tuning excitonic anisotropy in orthorhombic GeS

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Monochalcogenides, Germanium sulfide (GeS) is considered a promising material in optoelectronics applications due to its high optical absorption and optical band gap (BG) in the visible range, which can be effectively tuned by applying an external strain. This allows for modulation of its emission wavelength. GeS also exhibits high photosensitivity, a broad spectral giant piezoelectricity of response. and because its characteristic "puckered" symmetry. То fullv explore exciton-based applications and improve their performance, it is essential to understand the exciton behavior in anisotropic materials. In our work, we investigate the optical properties of anisotropic excitons in GeS encapsulated by h-BN using polarizationdifferent approaches that combine and temperature-dependent photoluminescence (PL) measurements, ab initio calculations, and effective mass approximation (EMA). Using the Bethe-Salpeter Equation (BSE) method, we found that the optical absorption spectra in GeS are significantly affected by the Coulomb interaction included in the BSE method, which shows the importance of excitonic effects besides it exhibits a significant dependence on the direction of polarization, revealing the anisotropic nature of bulk GeS. By combining ab initio calculations and EMA methods, we investigated the quasi-hydrogenic exciton states and oscillator strength (OS) of GeS along the zigzag and armchair axes. We found that the anisotropy induces lifting of the degeneracy and mixing of the excitonic states in GeS, which results in highly non-hydrogenic features. A very good agreement with the experiment is observed.

[P12] First principle study of an anti-gout molecule Allopurinol and its dimer: A quantum chemical approach

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The electronic characteristics. vibrational modes. time-dependent excitation features like TDDFT (Time-dependent density functional theory) in gas and DMSO (Dimethyl sulfoxide) solvents, charge distribution via NBO (Natural bond orbitals) analysis, and particular biological profiles of allopurinol and its dimer are all examined in this work using the DFT/B3LYP method with the 6-311G (d, p) basis set. In energy calculations, dimers with long-range interactions are studied using the wB97XD functional. HOMO molecular orbital). LUMO (highest occupied (lowest unoccupied molecular orbital), and MESP graphs are used to determine the electronic characteristics of the title molecule's monomer and dimer. In comparison to the B3LYP function, the computational results show that wB97XD overestimates the energy gaps for the monomer and dimer by 91% and 83%, respectively. The molecule's observed UV spectra are contrasted with those calculated with the wB97XD functional in methanol. The most stable dimer generated by N5-H26 (3.95 kcal/mol) and N15-H14 (5.65 kcal/mol) has hydrogen bonding, according to study using the Quantum Theory of Atoms in Molecules (QATIM). NBO analysis demonstrates that the np $\rightarrow \sigma^*$ interaction mediates the interaction between two dimer units. The chemical in the title has shown great promise in treating gout. The chemical has a high affinity for the XDH (Xanthine Dehydrogenase) protein, according to the FF score and binding affinity.

Keywords: DFT, NBO, HOMO, LUMO, XDH

[P13] Exploring photovoltaic potential of CZTS: An abi initio study of kesteric solid solutions

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CZTS (copper-zinc-tin-sulfide) is being extensively studied as an alternative to CIGS (copper-indium-gallium-selenide) for thin film solar cell applications. This interest is due to the greater abundance of the elemental components of CZTS in the Earth's crust compared to CIGS. Additionally, CZTS has a crystal structure similar to chalcopyrite with a slightly different (space group of kesterite, I-4), and is thus expected to have comparable properties.

Like chalcopyrites, kesterites can form solid solutions that influence their electronic and photovoltaic properties. Investigating this impact is essential to predict the potential of a specific kesteritic material for photovoltaic applications.

We conducted an ab initio study of kesteritic solid solutions relevant to photovoltaic applications and calculated their electronic properties. Additionally, we performed many-body perturbation theory (MBPT) calculations to obtain absorption spectra and analyze their dependence on elemental concentrations. Special attention was given to including excitonic effects in the calculations and evaluating their impact on the final spectra.

For the initial density functional theory (DFT) computation, we used the plane-wave-based pw.x utility from Quantum Espresso. The resulting wave functions were subsequently used in MBPT calculations with the Yambo code, where excitonic effects were modeled using the Bethe-Salpeter equation.

We successfully predict the optical absorption and electronic structure of the given kesteritic materials, and hence our results enhance the understanding of this class of materials and could significantly contribute to future solar cell design.

[P14] Layer-number and strain effects on the structural and electronic properties of PtSe2 material

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For the past decade, platinum diselenide (PtSe2) has exhibited remarkable physical properties, such as high electron mobility, air stability [1], and the ability to emit in the THz range. Additionally, its bandgap varies with the number of layers, revealing a transition from semiconductor to semimetallic as the thickness increases. In our work, density functional theory (DFT) with various van der Waals (vdW) corrections was used to study the effect of the number of layers on the structural and properties of PtSe2. The vdW corrections electronic considered yielded different results regarding the number of layers at which the semiconductor-to-semimetal transition (SM-SC) occurs. This variation is attributed to the different interlayer distances observed for each correction, highlighting the sensitivity of the bandgap to this distance, in addition to the number of layers. In fact, the bandgap increases with the interlayer distance due to the energy shift of the conduction and valence bands dominated by Se-pz orbitals. According to comparisons with available experimental data, the vdW-DF and rVV10 corrections provided the most accurate results. Furthermore, controlling the interlayer distance through vertical compressive strain allowed for the modulation of the bandgap in bilayer PtSe2. A semimetallic character for bilayer PtSe2 can indeed be achieved under a vertical strain of 17%. Our work demonstrates a deep understanding of the correlation

between structural and electronic properties, as well as the potential to tune the bandgap through the application of strain. For our future research, we aim to investigate the electronic and optical properties of monolayer PtSe2 under the influence of an external electric field. This study will offer insights into the ability to adjust these properties for different technological applications.

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[P15] Thermoelectric properties and optical response of the main species present in Portland cement pastes

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Several experimental studies have been conducted on the thermoelectric properties of cementitious materials, but a detailed inspection of the intrinsic properties of their main ingredients is still missing. This work focuses on the thermoelectric properties of portlandite and tobermorite, two mineral components found in Ordinary Portland Cement pastes. To this end, atomistic simulations were carried out to predict the thermoelectric properties and optical response of cement-based materials. The methodology is based on the functional approach densitv theory together with GW-guasiparticle, Bethe-Salpeter equations, and Boltzmann transport equation methods. As expected, the undoped minerals have low thermal conductivity. However, both the Seebeck coefficient and the electrical conductivity can be dramatically increased by appropriate carrier doping. In fact, an enhanced figure of merit of Z = 0.6 at 650 K and 0.79 at 600 K is observed for portlandite and tobermorite. Therefore, our results confirm that there are still much promising prospects for enhancing the characteristics of concrete materials for energy harvesting.

[P16] Green's function methods towards the exascale

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Materials are crucial to science and technology, and connected to major societal challenges ranging from energy and environment. to information. communication. and The manufacturing. accuracy efficiencv and of electronic-structure methods are driving a new paradigm in research. With simulations becoming increasingly faster and efficient, they serve as indispensable tools for understanding, predicting and designing material properties. Many-body perturbation theory (MBPT) and Green's function methods offer an accurate description of excited electrons. However, these approaches come with significant computational cost. Conventional GW implementations have a computational cost that scales as $O(N^4)$ with respect to the system size N, limiting the scope of GW calculations.

The efficiency of electronic-structure calculations depends both on the development of computational algorithms and hardware technology. Here we present new algorithm developments recently implemented in the Yambo code [1,2], aiming at improving accuracy and efficiency, such as the W-av method [3] and the multi-pole approximation (MPA) [4,5] as well as a new python software layer (Yambopy) able to perform post-processing operations and manage Yambo workflows.

In the effort of improving hardware performance, solutions based only on many-cores architectures are being

conspicuously replaced by heterogeneous or accelerated architectures. We will discuss the strategy devised for the GPU porting of the Yambo code, as well as the resulting speedup of the calculations. Yambo is now able to efficiently run on all presently available accelerated machines in Europe, alternatively adopting CUDA-Fortran, OpenACC, and OpenMP offloading programming models.



Figure: Calculation of quasi-particle corrections on a graphene/Co interface. On the left, the scalability test on Leonardo-Booster (CINECA), while at the right a speedup comparison between Leonardo-DCGP, Leonardo-Booster and LUMI-G (CSC) for the same system but with reduced parameters.

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[P17] High-Harmonic Generation in Periodically Driven Systems: A Floquet-Fourier Approach

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High-harmonic generation (HHG) in solid-state systems offers critical insights into ultrafast electron dynamics and potential applications in ultrafast photonics [3]. We investigate HHG in a one-dimensional electron chain subject to a staggered potential, modeling essential aspects of charge density wave (CDW) ordered materials under illumination bv а monochromatic laser field. Utilizing Floquet theory, which leverages the time periodicity of driven quantum systems, we derive an analytical formula to calculate the high-harmonic components (HHC) of the electric current when a laser field is switched on Floquet theory treats the time-dependent Schrödinger equation by defining guasienergies, analogous to quasimomenta in spatially periodic Bloch systems [1]. Using this framework, we show analytically the emergence of two distinct plateau regions in the HHG spectrum. The widths of these plateaus scale linearly with the electric field amplitude but inversely with the laser frequency and its square, respectively. indicating different underlying physical mechanisms. Numerical simulations further reveal multi-step plateau structures appearing under strong electric fields and potentials, reflecting significant staggered complex electron-lattice interactions.

Our analytical and numerical results align closely with a previous study [2], confirming the robustness of the Floquet-Fourier method. This approach can readily be

generalized beyond one-dimensional systems, enabling the of HHG phenomena in higher-dimensional exploration materials and allowing the incorporation of additional complex interactions such as spin-orbit coupling (SOC), Rashba effects, electron-electron interactions, and electron-phonon coupling. These findings provide new insights into controlling HHG in periodic potentials, highlighting possibilities for tailoring electronic in optoelectronic and responses quantum technologies. The clear understanding of plateau structures and their scaling behavior under varying field strengths and frequencies contributes significantly to advancing ultrafast spectroscopy and coherent extreme-ultraviolet radiation generation.



Figure 1: The HHC spectrum in the single-band limit for a 1D system. Each data set corresponds to the field strength F = 0.1 (blue), 1.0 (orange), 5.0 (green), and 8.0 (red). The ω refers to the frequency of the laser light and Q is the value of the staggreed potential.

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[P18] Monolayer silicene grown on Ag2X surface alloys (X=Sn, Ge, Sb, Pb and Bi): A first-principles study

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Silver (111) is one of the most studied substrates for arowing monolayer silicene. Specifically, the formation of various silicene reconstructions (4×4, $\sqrt{13}\times\sqrt{13}R13.9^\circ$ type I and II, $2\sqrt{3}\times 2\sqrt{3}R30^\circ$, and others) has been observed[1–3], yielding to polycrystalline samples, which in turn introduces scattering centers for charge carriers. It is instead crucial to synthesize large-scale, misorientation-free single crystals of monolayer silicene. Previous experiments have demonstrated that monolayer silicene of nearly isolated form, with a sample size of the cm² scale, can be successfully grown on Ag2Sn/Ag(111) via molecular beam epitaxy (MBE) [4]. This process has been well-supported by theoretical calculations [4], highlighting the potential of a decoupled silicene layer on a single-elementdecorated Ag(111) surface. We extend these studies and explore the feasibility of forming monolayer silicene on Ag2X surface alloys on Ag(111), where X represents different doping elements (Sn, Ge, Sb, Pb, and Bi). Based on density functional theory (DFT) as implemented in Quantum Espresso software, we examine the equilibrium adsorption structures, silicene buckling, adsorption energies, charge transfer, and electronic properties of silicene on Ag2X/Ag(111) substrates. We considered three types of silicene superstructures, namely $(4\times4, \sqrt{13}\times\sqrt{13}, \text{ and } \sqrt{3}\times\sqrt{3})$ [1–3], that require different superlattices of Ag(111) $(4\sqrt{3}\times 4\sqrt{3}, \sqrt{39}\times \sqrt{39}, \text{ and } 2\sqrt{3}\times 2\sqrt{3}).$

Our results show that the buckling increases with doping, following the order: Ge, Sb(Sn), Pb, and Bi. Regarding the strength of the Si-substrate interaction, the trend is approximately reversed. These findings suggest that silicene on Bi, Sb, and Pb-doped superlattices is more feasible to form decoupled silicene compared to that on Sn- and Ge-doped superlattices. Furthermore, charge transfer analysis reveals that for Sn-doped superlattices, minimal charge transfer occurs from silicene to the substrate, while for Ge-doped systems, the charge transfer is considerably larger yet still smaller than on pristine Ag(111). Finally, we investigated the electronic structures of silicene upon adsorption on the Ag2X/Ag(111) substrates. Our study offers valuable insights that could guide experimental efforts in the synthesis of high-quality, decoupled silicene monolayers, which are essential for the advancement of future nanoelectronic devices based on this material.

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[P19] CrSBr: A Layered Magnetic Semiconductor with Strong Excitonic Effects

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The CrSBr van der Waals layered material is a magnetic semiconductor which has gained attention due to its unique magnetic and optical properties. It is air-stable and allows for manipulation of its magnetic order with a small external field, positioning it as a promising candidate for magnonics applications. In this context, CrSBr may enable energy-efficient information transfer through coherent magnons. Information about these low-energy magnetic excitations could potentially be accessed optically through their coupling with excitons, possess higher excitation energies, making which the exciton-magnon interaction an active area of research. As part of this year's Yambo School, we present our recent first-principles studies of CrSBr, combining ground-state density functional theory with excited-state many-body perturbation theory. In particular, we investigate the excitonic effects using the Bethe-Salpeter equation, and analyze how these are influenced by the underlying magnetic configuration. Future research will explore ultrafast excitonic dynamics and its interplay with magnetism using real-time simulations.

[P20] Stacking-Dependent Interlayer Excitons in BP/CrSe2 van der Waals Heterostructure

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The emergence of two-dimensional van der Waals (vdW) heterostructures has revolutionized

exciton-based research due to their tunable electronic and optical properties. Here, we present a systematic many-body study of BP/CrSe2 vdW heterostructure composed of experimentally realized boron phosphide (BP) and chromium diselenide (CrSe2) monolayers. We find a robust type-II band all stacking configurations; however, across alignment interlayer excitons emerge selectively depending on the stacking order. The vdW heterostructure exhibits strong exciton binding energy of $\sim (0.3 - 0.5 \text{ eV} \text{ depending on})$ stacking) and nanosecond-scale room-temperature radiative lifetimes, indicating long-lived excitonic states. Additionally, its optical absorption extends from the visible to the near-infrared regime, underscoring its potential for optoelectronic and excitonic applications. Our findings highlight the critical role of stacking-dependent interlayer coupling in controlling the excitonic properties of vdW heterostructures, paving the way for tailored design strategies in next generation light-harvesting and quantum technologies.

[P21] Phase space exploration of Au^I-Au^{III} and Ag^I-Au^{III} double perovskites using ab initio calculations.

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Mixed-valence gold-based double perovskites, such as Cs₂Au^IAu^{III}I₆, have been proposed as promising lead-free alternatives for photovoltaic applications due to their predicted direct band gap, which is closer to the Shockley-Queisser limit than that of MAPbl₃ [1,2], their short-circuit current density, which is 2.5 times higher than that of MAPbl₃ [1], their polycrystalline thin films with high photoconversion efficiencies, and their two-dimensional excitonic behaviour [2]. However, to date, no efficient photovoltaic devices based on these materials have been realized. Recent studies on mixed-valence gold-based double perovskites often also of include comparative studies the isoelectronic silver-gold-based double perovskites, such as Cs₂Ag^IAg^{III}I₆, cost-effective which presented as and are more environmentally friendly alternatives. At room temperature, these compounds preferentially crystallize in the tetragonal 14/mmm space group [3], and the existence of a cubic F m 3m allotropic variety has been discussed [4]. It has recently been theorized that the photoluminescence properties of Cs₂Au^IAu^{III}I₆ could be affected by a phonon-induced process [5]. Could a similar process influence the photovoltaic performance of the material?

In this study, we consider the $Cs_2M^{I}Au^{III}I_6$ (M = Au, Ag) compounds, and investigate the relative stabilities of the two experimentally reported phases of both systems using

first-principles calculations. A key discovery of this study is that, in both systems, the tetragonal phases are energetically favored and dynamically stable, thus suggesting that the cubic structure is metastable. Additionally, we identify a credible origin for the poor performance of photovoltaic devices, in agreement with experimental observations [4,5]. Specifically, the F m⁻³m phases are metallic, and if small clusters of them were to form, they would act as traps for charge carriers, thereby severely impairing the photovoltaic performance of the devices. Future work will focus on the optoelectronic properties of these materials to further assess their viability for photovoltaic applications.

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[P22] Modulating Spin States and Magnetic Properties in Molecular Adsorbates on Crl3 for Spintronic Applications

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spintronics, In the realm of molecular molecular semiconductors offer a versatile platform enriched with mechanical flexibility, photovoltaic prowess, ferroelectric magnetic exchange interactions [1-3]. and properties. Complementing this, the magnetic behavior of 2D magnet Crl3 is scrutinized for its layer-dependent characteristics, shedding interlayer interactions and magnetic ordering liaht on mechanisms [4]. Our investigation delves into the interplay between spin states and iron phthalocyanine (FePc) molecules adsorbed onto defect-functionalized CrI3 substrates. We focus on three stable vacancy defects in Crl 3, created by the removal of '-Cr-', '-I-', and '-Crl3-' units from the pristine lattice, analyzing their electronic and magnetic characteristics in both FM and AFM scenarios via first-principle calculations. FePc demonstrates two stable spin states: a 2 µB low-spin state and a 4 µB high-spin state. Two spin-control mechanisms emerge when FePc adsorbs onto these defect-functionalized substrates: substrate-induced and molecular spin vector-induced control [5]. These findings propose effective methods to control the spin states of magnetic metal complexes during adsorption onto magnetic substrates, enabling potential applications in molecular electronics and spintronics with 2D materials. Building on this, we study Nheterocyclic carbene (NHC) [6] molecules adsorbed on a Crl3. NHC adsorbs vertically with the electron rich carbene C above an I atom, lifting it from the substrate. This leads to charge loss on I, increased magnetic moments on Cr atoms originally bonded to it, and a net substrate moment increase of 2 µB per adsorbed molecule. We detect the emergence of two extra states. To complement our DFT work, we have initiated TD-DFT calculations to understand the excited-state behavior of the NHC-Crl system; however, to accurately capture guasiparticle₃ corrections and excitonic effects-and ultimately achieve our goal of exploring photo-responsive spintronic behavior in molecular-semiconductor/2D-magnet hybrids-we intend to go beyond TD-DFT [7] by employing many-body perturbation theory (GW and BSE), paving the way for novel opto-spintronics applications.

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[P23] Many-body study of quasiparticle and exciton dispersions, and optical excitations in high-efficiency solar materials

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We study charged and optical excitations in LiZnAS and ScAgC half-Heusler compounds for solar cell applications using first-principles-based density functional theory (DFT) and the many-body Bethe-Salpeter equation (BSE) calculations. By incorporating many-body electron-electron and electron-hole correlation effects into DFT-based calculations, we achieve a high-quality description of electronic and optical properties in both materials, with the obtained band gap falling within the desired range for solar applications. Our results for LiZnAS show agreement with previous strona experimental measurements, analyzed using various levels of theory used in our calculations. Optical absorption in both materials show strong peak in visible light region, making these to more efficient for photovoltaic applications. We also examine the exciton wave function in real and momentum space, offering key insights into the localization and delocalization nature of excitons at various peaks in the optical spectra, which is crucial for optimizing these materials for solar cells. Finally, we assess the solar efficiencies using the spectroscopic limited maximum efficiency (SLME) model, obtaining SLME values exceeding 30%, making these materials highly promising candidates for photovoltaic applications.