The Abdus Salam International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

Wannier 2022 Summer School | (SMR 3705)

16 May 2022 - 20 May 2022
ICTP, Trieste, Italy

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P01

Laser-induced charge and spin photocurrents in BiAg2 surface from first-principles

The physics of photo-induced effects in interfacial systems is intensively researched these days owing to numerous potential applications. Owing to the complexity of the problem, a comprehensive theoretical picture of photogalvanic effects taking place at realistic metallic surfaces and interfaces is still lacking. In the past, it was shown that in the ferromagnetic Rashba model with in-plane magnetization charge and spin photocurrents which are of second order in the electric field are allowed by symmetry. Additionally, second order spin photocurrents are allowed by symmetry in the non-magnetic Rashba model. These responses stem from the interfacial spin-orbit interaction (SOI) and can be generated by the application of femtosecond laser pulses [1,2]. Here, we report calculations of laser-induced currents within the Keldysh non-equilibrium formalism combined with the Wannier interpolation scheme which can be applied to metallic and insulating materials of any complexity. We perform our first-principles electronic structure calculations with the DFT code FLEUR www.flapw.de, and study in detail a BiAg2 surface, which is a well-known material realization of the Rashba model. The in-plane magnetization is introduced by the addition of a Zeeman splitting term in the Wannier-interpolated Hamiltonian. We calculate the laser-induced charge photocurrents for the ferromagnetic case and the laser-induced spin photocurrents for both the non-magnetic and the ferromagnetic case. Our results confirm the appearance of in-plane photocurrents as predicted by the Rashba model. The resulting photocurrents satisfy all the predicted symmetry restrictions with respect to the light helicity and the magnetization direction. We provide microscopic insights into the symmetry and magnitude of the computed currents based on the electronic structure of the system. Our work contributes to the study of the role of the interfacial Rashba SOI as a mechanism for the generation of in-plane photocurrents, which are of great interest in the field of ultrafast and terahertz spintronics. [1] F. Freimuth, S. Blügel, and Y. Mokrousov, Phys. Rev. B 103, 075428 (2021). [2] F. Freimuth, S. Blügel, and Y. Mokrousov, Phys. Rev. B 94, 144432 (2016).

P02

Fe2MnSn Heusler alloy: A comprehensive study

Heusler alloys are an exciting class of materials, offering a huge compositional space for the search of rare earth free permanent magnet and also for spintronics applications. In this regard, the Fe based Heusler alloy are particularly more fascinating because of its earth's abundance, large magnetic moment and a relatively high Curie temperature. We perform first principles density functional theory calculations to study the thermodynamic phase stability, electronic and magnetic properties of Fe2MnSn Heusler alloys. Taking into account of all different structural phases viz. XX, XX, XXX, YY, and YYY, we identify the lowest energy structure by taking into account of explicit spin-spin interaction, spin-orbit interaction as well as free energy of vibration. Thereby, the ferromagnetic hexagonal (D019) phase, with high magnetization of ~6.45 μB/f.u. and a sizable magneto-crystalline anisotropy energy of ~1.28 MJ/m3, is found to be the magnetic ground state. Further, for this particular phase the exchange coupling constants between the different magnetic ions are calculated from Liechtenstein approach within the KKR-Green functions formalism. The Curie temperature is estimated to be Tc = 542.3 K using the mean field approximation.

P03

A position-dependent ab initio tight-binding model for twisted TMD bilayers

The discovery of superconducting and correlated insulating states in magic-angle twisted bilayer graphene has led to intense interest in other moiré materials. Twisted bilayer transition metal dichalcogenides (TMDs), for example, have been shown to exhibit correlated insulating states at different fillings, possible superconducting behaviour [1], and exotic optical properties [2]. The large size of the moiré unit cells of small-angle twisted TMD bilayers renders electronic structure calculations based on density functional theory (DFT) unsuitable for the routine study and exploration of their large chemical and structural phase space. Therefore, atomistic tight-binding models are often used. Whilst tight-binding models with position-dependent interlayer hoppings have been developed, a model that captures position dependence within a layer doesn't exist. This is essential to describe the effect of intralayer atomic relaxations on the emergence and nature of flat bands in the electronic structure [3], as well as to calculate electron-phonon coupling. In this work, we develop a position-dependent intralayer TMD tight-binding Hamiltonian. Our model is based on Slater-Koster relations that are parametrized to hoppings obtained from first-principles DFT Hamiltonians of strained monolayer TMDs in a basis of maximally localized Wannier functions. [1] Wang L. et al., Nat. Mat. 19, pages 861–866 (2020) [2] Tran, K., et al., Nature 567, 71–75 (2019) [3] Li, H., et al., Nat. Mater. 20, 945–950 (2021)

P04

Wannier interpolated band structure of $CsPbCl_3$ perovskite

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Lead halide perovskites $CsPbX_3$ (X is a halogen) are potential candidates for photovoltaic technology due to their efficiency, low cost and easy fabrication procedure. The key property of these materials is the band gap energy, which must be determined precisely. In this work the ground state structure and the electronic properties of the $CsPbCl_3$ perovskite are investigated with DFT as implemented in the Quantum Espresso package. The PBE-GGA approximation is used for the exchange-correlation term. The band structure is calculated with the HSE hybrid functional through Wannier90 code. The obtained band gap energy is about 3.16 eV, which is in good agreement with experimental data.

Keywords: Perovskites; Band gap; HSE; Quantum Espresso; Wannier.

P05

Ab initio phonon self-energies: To screen, or not to screen

Authors: Jan Berges, Nina Girotto, Tim Wehling, Nicola Marzari, Samuel Poncé First-principles calculations of phonons are often done under the adiabatic approximation and using a sparse Brillouin-zone sampling. These shortcomings can be remedied through corrections to the phonon self-energy from the low-energy electrons, responsible for adiabatic and nonadiabatic Kohn anomalies. A well-founded correction method exists [Calandra, Profeta, and Mauri, Phys. Rev. B 82, 165111 (2010)], which only relies on readily available (adiabatically) screened quantities. However, perturbation theory suggests to use one bare electron–phonon vertex in the phonon self-energy [Giustino, Rev. Mod. Phys. 89, 015003 (2017)] to avoid a double counting. A possible middle way is based on downfolding to partially screened phonons and interactions [Nomura and Arita, Phys. Rev. B 92, 245108 (2015)]. In this work, we compare these approaches by means of numerical calculations for TaS_2, n-doped MoS_2, B-doped diamond, and MgB_2 and by revisiting the underlying formulas, thus addressing a recent controversy about the correct screening of the electron–phonon interaction in phonon self-energies [Paleari and Marini, arXiv:2105.09823].

P06

Spin Dependent Tunneling of All Heusler alloy Junction

Magnetic tunneling junction (MTJ) is the backbone of many spintronics devices, which enables the function of random access memory devices, spin transfer torque devices\cite{Ralph} and next generation neuromorphic computing. MTJ devices, consisting of two ferromagnetic electrodes separated by a non-magnetic insulator, have been the subject of intense research in the recent years. In these devices the tunneling magnetoresistsnce (TMR) are strongly dependent on the relative spin orientations of both the electrodes (parallel or anti-parallel), which gives the TMR devices the flexibility of electric readout of the magnetically stored information. Therefore, in this work, we address the following question: given all these varieties of properties in the Heusler alloy class, is it possible to create an full-half Heusler based magnetic tunneling junction alternative to full Heusler/MgO based junctions ? Our analysis focuses on the spin dependent transmission properties of the all Heusler alloy Junction. We have further probed the robustness of the Half metallic behavior at the interface with respect to the various atomic diffusion and defects.

P07

Structural and electronic properties of Eu-doped $CsGeCl_3$ perovskite

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Recently, a great deal of interest has been developed in doping inorganic lead halide perovskites with rare earths. Due to the toxic effect of lead, development of novel, environmentally friendly and sustainable energy storage devices have attracted considerable research attention. Focusing on the toxic effect of the lead, many experimental studies have been carried out to substitute the lead by tin and germanium and/or by doping with transition metals or rare earth elements. In this work we investigate the effect of Eu doping effect on the structural and electronic properties of $CsGeCl_3$ perovskite by using the DFT method combined with the Quantum Espresso package.To evaluate precisely the band gap energy, the HSE hybrid functional is adopted through wannier90 package. The geometrical stability, structural parameters as well as the band gap energy are studied as a function of Eu-content.

Keywords: Photovoltaic materials ; perovskite structure ; DFT ; HSE ; Quantum Espresso ; Band gap ; wannier90 .

P08

Hexagonal SiGe as a direct-gap semiconductor

The indirect band gaps of diamond-structured Si and Ge make them inefficient light emitters, limiting their application in active photonic devices (e.g. light-emitting diodes and lasers). Realising Si-compatible direct-gap semiconductors to provide a key enabling technology for Si photonics has therefore attracted attention for several decades. While progress has been made via monolithic integration of III-V semiconductors on Si, this presents significant challenges for epitaxy and device thermal management. In recent years there has therefore been a surge of interest in approaches to achieve direct-gap group-IV semiconductors via band structure engineering. Advancements in materials growth now allow Ge and Si nanowires to be fabricated reproducibly and with high crystalline quality in the lonsdaleite ("hexagonal diamond") phase. Recent experimental measurements have demonstrated impressive optical properties in lonsdaleite SiGe alloy nanowires, distinguishing hexagonal group-IV semiconductors as a promising platform for the development of Si-compatible photonic devices. From a theoretical perspective, it is well known that lonsdaleite Ge and Si are respectively direct- and indirect-gap semiconductors. This suggests the possibility to achieve Ge-rich SiGe alloys having a direct band gap. However, the direct band gap in lonsdaleite Ge originates via back-folding of the L-point conduction band minimum of diamond-structured Ge, leading to a "pseudo-direct" band gap with weak oscillator strength. We present a detailed first principles analysis of the electronic and optical properties of lonsdaleite SiGe alloys, elucidate the electronic structure evolution and direct- to indirect-gap transition, and describe the important impact of alloy band mixing effects on inter-band optical transition strengths.

P09

Berry Curvature dipole senses topological phase transition in a moir\'{e} superlattice

The interplay of topological aspects of electron wavefunction and crystalline symmetry can lead to different physical properties of materials. Berry curvature and Chern number are two characteristic features of electronic bands that are used to define the topological nature of any system. While Berry curvature and its effects in materials have been studied, detecting changes in the topological invariant, Chern number, is challenging. In this regard, twisted double bilayer graphene (TDBG) has emerged as a promising platform to gain electrical control over the Berry curvature hotspots and the valley Chern numbers of its flat bands. In addition, strain induced breaking of the three-fold rotation symmetry in TDBG, leads to a non-zero first moment of Berry curvature called the Berry curvature dipole (BCD), which can be sensed using nonlinear Hall (NLH) effect. We reveal, using TDBG, that the BCD detects topological transitions in the bands and changes its sign. In TDBG, the perpendicular electric field tunes the valley Chern number and the BCD simultaneously providing us with a tunable system to probe the physics of topological transitions.

P10

Peierls distortion and electronic transport in exfoliable novel 1D materials

Low-dimensional materials have seen intense research in the last decades due to their unique electronic properties and the great potentialities in next-generation applications. 1D systems for example, despite poorly investigated, are extremely promising for many applications in electronics, optoelectronics and energy storage. Following the work of Mounet et all., a high-throughput screening has been performed to discover new promising 1D materials that could be isolated from their VdW parents, finding more than 800 1D or quasi-1D wires. Here, we characterise novel 1D metallic chains selected from this portfolio for the high density of state at Ef, as possible candidates for electronic devices. Low-dimensional materials are well-know for their dynamical instabilities, which bring to structural phase transition of the lattice at nonzero wavevector, such as Peierls distortion and charge density waves (CDW). We pay particular attention on the structural stability of the chains, inspecting the DFPT-phonon dispersion in order to reconstruct the supercell at qCDW and identify the stable systems in metallic phase.

P11

Koopmans spectral functionals in periodic-boundary condition

Koopmans spectral functionals aim to describe simultaneously ground state properties and charged excitations of atoms, molecules, nanostructures and periodic crystals. This is achieved by augmenting standard density functionals with simple but physically motivated orbital-density-dependent corrections. These corrections act on a set of localized orbitals that, in periodic systems, resemble maximally localized Wannier functions. At variance with the original, direct supercell implementation [{\it Phys. Rev. X} {\bf 8}, 021051 (2018)], we discuss here i) the complex but efficient formalism required for a periodic-boundary code using explicit Brillouin zone sampling, and ii) the calculation of the screened Koopmans corrections with density-functional perturbation theory. The implementation in the Quantum ESPRESSO distribution and the application to prototypical insulating and semiconducting systems are presented and discussed.

P12

Interplay between structural deformations and flat band phenomenology in twisted bilayer antimonene

In this work we apply first principles calculations to investigate the flat band phenomenology in twisted antimonene bilayer. We show that the relatively strong interlayer interactions which characterize this compound have profound effects in the emergence and properties of the flat bands. Specifically, when the moiré length becomes large enough to create well defined stacking patterns along the structure, out-of-plane displacements take place and are stabilized in the regions dominated by the AB stacking, leading to the emergence of flat bands. The interplay between structural and electronic properties allows for detection of flat bands in higher twist angles comparable to other two-dimensional materials. We also show that their energy position may be modulated by noncovalent functionalization with electron acceptor molecules.

P13

Superconductivity of atomic hydrogen at high pressures

Atomic hydrogen is expected to have the highest critical temperature of all conventional superconductors. A recent study showed the importance of including quantum anharmonic effects for stabilizing this hydrogen structure. Here we will try to investigate the influence of the quantum anharmonic effects on the superconductivity properties of atomic hydrogen. In accordance with the previous study, we find that the inclusion of the quantum effects leads to the in-plane lattice parameter compression and the increase of the c/a radius of the tetragonal structure of atomic hydrogen. This in turn softens the acoustic phonons frequencies and stiffens the optical phonon frequencies. Furthermore, the electronic density of states at the Fermi level is increased in the structures with quantum effects. We interpolate the electronic and vibrational properties of these structures using Wannier functions in order to get a reliable estimate of the critical temperature in this system.

P14

Collective plasmonic modes in the chiral multifold fermionic material CoSi

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Abstract: Plasmonics in topological semimetals offers exciting opportunities for fundamental physics exploration as well as for technological applications. Here, we investigate plasmons in the exemplar chiral crystal CoSi, which hosts a variety of multifold fermionic excitations. By using realistic Wannier function-based tight-binding modeling, we calculate the dielectric function within random-phase approximation. We show that CoSi hosts two distinct plasmon modes in the infrared regime at 0.1 eV and 1.1 eV in the long-wavelength limit. The 0.1 eV plasmon is found to be highly dispersive, and originates from intraband collective oscillations associated with a double spin-1 excitation, while the 1.1 eV plasmon is dispersionless and it involves interband correlations. Both plasmon modes lie outside the particle-hole continuum and possess long lifetime. Our study indicates that the CoSi class of materials will provide an interesting materials platform for exploring fundamental and technological aspects of topological plasmonics.

P15

Modelmaker: An automated second-principles model generator

In the last decades advances in computation, using first principles methods such as Density-Functional-Theory (DFT), have allowed improving our understanding of electronic structure of all kinds of materials. However, the study of properties beyond the ground state using these methods, as well as taking into account the effects of temperature is still very limited. In recent years a new family of techniques based on DFT, known as Second Principles (SP) [Phys. Rev.B 93, 195137 (2016)], have been developed to solve these difficulties. They allow large-scale simulations in materials including both vibrational and electronic degrees of freedom, at a very modest computational cost. Its practical application requires the construction of models written in a basis set of localized functions: The Wannier basis set, obtained for each particular system using WANNIER90. In this work, we establish a general method to systematically obtain the parameters of SP models from DFT, with the goal of predicting the conductivities and optical properties of a wide set of materials that go from conventional metallic and insulating structures, to graphene and other systems that display non-trivial topological band structures. The simulation of these phenomena requires accounting for changes in electronic state (electronic density) and geometry. Therefore, the models are set as an extension of tight binding one-electron models including also electron-electron and electron-phonon interactions, needed to describe transport or magnetic properties in real materials.

P16

Chiral magnetism, phonons, and anomalous Hall conductivity in the novel antiferromagnetic antiperovskite

Chiral antiferromagnetic antiperovskites, where a magnetically active 3d metal cation is placed in the octahedral corners, are in the spotlight due to their intertwined magnetic structure and topological properties. Especially, their large anomalous Hall conductivity and the ability to be controlled by applied strain and/or electric field make them highly attractive in the condensed matter field. Herewith, we present the study and understanding of an unexplored antiperovskite compound that can offer enormous opportunities from the technological and theoretical point of view. Therefore, we investigated, by theoretical first-principles calculations, the structure, magnetic ordering, and electronic behavior in the Vanadium-based antiperovskite. We found an N-centered antiperovskite structure as a ground state similar to the Mn3AN family. In such a phase, a Pm3m ground state was found in contrast to the Cmcm post-antiperovskite layered structure, as in the V3AN, A = Ga, Ge, As, and P. The dynamical and electronic properties of this antiperovskite were studied demonstrating its vibrational stability in the cubic structure and noncollinear magnetic ordering. Finally, we found that the topologically associated properties, and specifically, the anomalous Hall conductivity is one of the largest reported among the antiperovskites compounds.

P17

Overcoming the asymmetry of the electron and hole doping for magnetic transitions in bilayer CrI3

Electrical control of magnetism has great potential for low-power spintronics applications and the newly discovered two-dimensional van-der-Waals magnetic materials are promising systems for this type of applications. In fact, it has been recently shown experimentally (Jiang et al. 2018 Nat. Nanotechnol. 13, 549–553) that upon electrostatic doping by electrons bilayer CrI3 undergoes an antiferromagnetic-ferromagnetic (AFM-FM) phase transition, even in the absence of magnetic field. Doping by holes, on the other hand, does not induce the same transition in the experiment, which points to an intrinsic asymmetry in the hole and electron doping that limits the control of the transition by doping. We here show, based on first-principles calculations, that the asymmetry originates in the relativistic nature of the valence-band-edge states of the pristine bilayer, which inhibits the magnetic transition upon hole doping. Based on this finding, we propose an approach to overcome the asymmetry and predict the existence of the AFM-FM transition for both hole and electron doping upon moderate uniaxial compression along the soft direction of the bilayer.

P18

Nonadiabatic effects in graphene-based materials

The discovery of self-standing graphene prompted a search for other quasi two dimensional materials with similarly interesting features. Low dimensionality allows for some prominent features to be, not only tailored easily, but also for new physics to emerge. Modifying electron-phonon interaction or electron correlations by means of, e.g., strain and doping, could also induce one of the most desirable features - superconductivity. A well established method for calculating phonon dynamics is density functional perturbation theory, which relies on the adiabatic Born - Oppenheimer approximation, assuming the phonon dynamics to be energetically incomparable to electronic transitions. However, here we carry out an analysis of electron-phonon properties in highly-doped graphene, hole-doped graphane, electron doped molybdenum disulfide and arsenene and hole-doped indium selenide, where the static approximation fails and the importance of including dynamical corrections is undisputable. Nonadiabatic renormalization greatly modifies the electron-phonon coupling strength, which in turn impacts the superconducting transition temperature. Care should be taken when neglecting dynamical corrections as they have a quantitative and qualitative effect in predicting and understanding physical properties.

P19

Tunable Surface Plasmon Polaritons in Graphene/Boron Nitride van der Waals Heterestructures

Electromagnetic modes representing collective charge density oscillations localized on surfaces of 2D layers (surface plasmons) and their coupling with incident photons, leading to the formation of surface plasmon polaritons (SPPs), have been extensively researched in graphene. However with the recent advent of simple wafer-transfer techniques the opportunity to synthesise a vast number of quasi-2D layered metamaterials, known as van der Waals heterostructures has left a perceptible gap in both theoretical and experimental studies of their optical properties. In this work we calculated the excitation spectra of p(TM) polarized modes, for several layer combinations of pristine and electrostatically doped graphene/boron nitride heterostructures on a Al2O3 substrate. We present an extended 2D model (based on our previous work) for the prediction of response due to an external electromagnetic field in van der Waals heterostructures from first principles. Furthermore, we validate our model against a state-of-the-art method, in which we solve the RPA Dyson equation where the interaction between current fluctuations (described by a microscopic conductivity tensor) in the plane-wave electron subsystem is mediated by a photon propagator. Consequently, we have identified Dirac and out-of-plane acoustic SPP branches in the long-wavelength limit, whose dispersion was shown to be easily tuneable by varying the number of layers in the heterostructure. As a means to bridge the momentum gap between the evanescent SPP modes and infrared photons, we also explored the effect of patterning the topmost heterostructure layer of graphene into nanoribbons, which introduces symmetry breaking and leads to the formation of optically active Bloch plasmon modes.

P20

Hubbard-corrected density-functional-theory in 2D magnetic materials

Two-dimensional magnetic materials offer new possibilities in applications such as Van-der-Waals heterostructures which allows for the observation of novel and exotic effects within the ultrathin limit. Therefore, understanding and studying their ground state properties are of great importance. Here we present our computational study of electronic and vibrational properties of two-dimensional magnetic systems, a ferromagnetic and an antiferromagnetic monolayer (CrI_3 and FePS_3), by means of extended Hubbard-corrected density-functional-theory. The Hubbard parameters calculated by density-functional-perturbation-theory, have been considered to treat the localized electrons in d orbitals. Our results show particularly in the case of FePS3 the Hubbard parameters play an important role to well describe the ground state properties of the 2D magnetic system.

P21

Giant and tunneling magnetoresistance in unconventional collinear antiferromagnets with nonrelativistic spin-momentum coupling

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Magnetoresistance effects of multilayer structures with ferromagnetic electrodes are used in commercial spintronics devices. The effects rely on spin current generated by the time-reversal broken band structure of the ferromagnets. Realizing the counterpart effects in structures with all-antiferromagnetic electrodes remained hitherto experimentally elusive, as the conventional antiferromagnets exhibit symmetries that combine time-reversal with translation or inversion and thus prohibit nonrelativistic spin polarized bands and spin currents. Recently, we have predicted large magnetoresistance effects[1,2] in multilayers with unconventional antiferromagnets (see Figure) which break these combined time-reversal symmetries[3,4,5]. The opposite spin sublattices in the unconventional antiferromagnets are connected by nonrelativistic rotational symmetries, resulting in nonrelativistic spin-momentum coupling which alternates in the Brillouin zone but integrates to zero net magnetization (see Figure inset)[1,5]. In the present contribution, we will describe in detail mechanisms for the giant and tunneling magnetoresistance effects in unconventional antiferromagnets[1]. We will explain, based on our minimal models, that a large signal can be attributed to archetype features in the band structures, such as spin-polarised valleys[1]. Finally, we will discuss material realizations based on recent first-principle and wannier functions based calculations[1,6,7].

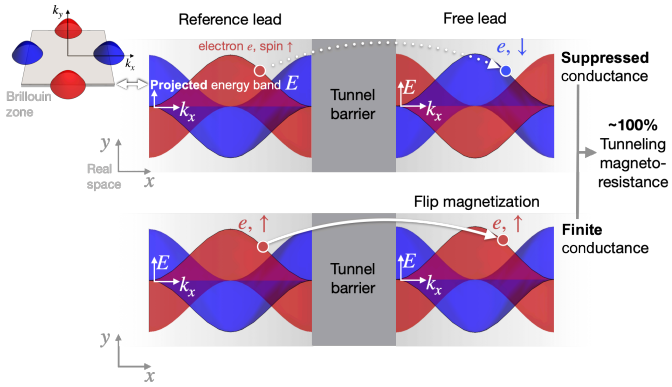

Figure 1: Large tunneling mangetoresitance ∼100% is found for a band structure with spin-polarized valleys where the opposite spin channels are separated in momentum space by large wave vectors.

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P22

Systematic study of magnetotransport responses within the Berry-Boltzmann formalism

There has been recently a huge renewed interest in the literature to the study of currents generated in solids by external electrical and magnetic fields. Different authors considered different models and different conditions and assigned different (sometimes confusing) names to various contributions to the current. The goal of this article is to bring order into the field, by systematizing the responses according to their properties with respect to the inversion and time-reversal symmetry. We perform a careful derivation of the formula for the current generated by electric and magnetic fields and classify the terms by their microscopic origin (classical, Berry curvature, Zeeman and Berry-Zeemann).

P23

Computing the band structure of two-dimensional electron systems in complex oxides using BinPo

After a high mobility two-dimensional electron system (2DES) was found at the LaAlO3/SrTiO3 interface, an intense effort in the oxide electronics community was done to unveil the underlying mechanisms, physical properties and feasible applications of such systems. Later on, many different procedures for creating a 2DES were revealed. Moreover, similar 2DESs were found in other complex oxides like KTaO3. In this context we present BinPo, an open-source Python code that allows for the calculations of the band structure in ABO3-based 2DESs. A general theory explaining the origin of the 2DES for all cases is still absent, however, our approach is independent of the microscopic origin of the charge carriers. BinPo computes the self-consistent potential energy in a slab system whose tight-binding Hamiltonian is created using a MLWF basis. The band structure, energy slices and other properties along with different projections and orientations can be computed. We gave priority to the ease-of-use and efficiency, in order to produce realistic simulations at low computational cost. We have benchmarked our band structure calculations with state-of-the-art ARPES measurements.

P24

Electronic band calculation of monolayer/bilayer WS_2: A Wannier90 study

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Two-dimensional (2D) transition metal dichalcogenides (TMDs) have attracted considerable interest owing to the possibility for next generation optoelectronic[1] and spintronic[2] devices. Manipulating these materials by unconventionally stacking them or intercalating with foreign atoms in the van der Waals heterostructure opens further possibilities for interesting physical phenomena and novel nanodevice applications. Recent advances in theoretical and experimental nanotechnology succeeded in stacking two or more layers of 2D materials with excellent control of twist angle in the relative orientation of the layers[3]. This new field of twistronics[4] further widened their application in controlling the electronic, optical and transport properties of 2D materials. For example, a graphene bilayer with a twist angle of $\sim 1.1^{o}$ exhibits flat bands leading to strong electron correlations and superconductivity[5] which are absent in the constituent monolayers.

In twisted TMD homobilayers such as WS_2/WS_2, the moiré bandwidth can be made arbitrarily small by reducing the twist angle, which produces strong correlation. Electrons or holes in these moiré bands are tightly localized in high-symmetry stacking regions, which can be well described by a simple effective tight-binding model. Wannier functions, which are composed by complete orthonormalized basis set, act as a bridge between a delocalized plane wave representation in electronic band calculations and a localized atomic orbital basis that describes chemical bonds. Interestingly, the recently developed Wannier tight-binding model can provide a computationally efficient way to predict electronic properties of materials[6].

To investigate the electronic properties of these fascinating 2D systems, we calculate electronic band structures for monolayer and weakly interacting twisted bilayers (AA and AB stacked) of WS_2, using the maximally localised Wannier functions based on density functional theory calculations by Quantum Espresso. Here, the band structures are constructed using $d_{z^2}, d_{xy}, d_{x^2-y^2}$ orbitals of tungsten atom and p_z orbital of sulphur atoms under the assumption that the valance and conduction bands have dominant contribution from these orbitals due to the symmetry of WS_2 monolayer.

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P25

Epitaxial growth, optical and electrical conductivity and electronic structure of the metallic pyrochlore Bi2Ru2O7 on Y-stabilized ZrO2 substrates

Epitaxial heterostructures composed of complex correlated metal oxides grown along unconventional crystallographic orientations offer a route to investigating emergent phenomena such as topological states and spin liquids through geometrical lattice engineering. We report on the epitaxial growth, structural and electrical properties of ordered, metallic pyrochlore bismuth ruthenate heterostructures grown along both the [001] and [111] directions. DC conductivity measurements together with optical transport parameters, which compare favorably with reported conductivity for the stoichiometric bulk compound, are also compared with calculated optical conductivity derived from density functional theory to gain insights into electronic behavior. Analysis of the magneto-transport parameters yield a carrier concentration that is in excess of the theoretical carrier concentration owing to Ru free electrons alone, and a low mobility confirming the presence of strong electron-electron interactions.

P26

Topology and oxidation states in ionic conductors

Recent theoretical advances, based on a combination of concepts from Thouless' topological theory of adiabatic charge transport and a newly introduced gauge-invariance principle for transport coefficients, have permitted to connect (and reconcile) Faraday's picture of ionic transport---whereby each atom carries a well-defined integer charge---with a rigorous quantum description of the electronic charge-density distribution, which hardly suggests its partition into well defined atomic contributions. We show that, by relaxing some general topological conditions, charge may be transported in ionic conductors without any net ionic displacements. As a significant byproduct, these results permit the classification of different regimes of ionic transport, according to the topological properties of the electronic structure of the conducting material.

P27

Title: First-principles investigation of topological properties in rare-earth-based materials and SnTe material class.

M. Ragargui

Abstract

Recently, topological insulators are at the focus of current research, with new concepts, new topological phases are rapidly discovered and proposed, in addition, the interplay of topology, and much internal symmetry give rise to propose the new topological crystalline insulators (TCI), where the topological conducting surface states are protected by spatial symmetry. These hold promise for game-changing applications in spintronic and nano-electronic. With their simple face-centered cubic structure and their richness of symmetries, many rare-earth monopnictides/nitrides can hold diverse electronic, magnetic, and topological proprieties. Here, using first-principles calculation by Quantum Espresso and tight-binding methods with maximally localized Wannier function basis implemented in Wannier90 and Wanniertools, this presentation will discuss the recent discoveries of topological propriety in rare-earth monopnictides/nitrides and an overview of topological crystalline materials, confirmed by our calculations. The band inversion and topological invariants in SnTe material are realized respectively, followed by the description of Dirac-like topological surface states in (001) surface of SnTe.

Keywords : Topological insulators, topological crystalline materials topological invariants, Wannier charge centers, DFT, Wannier90, Wanniertools.

P28

Characterization of topological semimetals with all-electron WIEN2k code

WloopPHI is a Python module that expands the features of WIEN2k, a full-potential all-electron density functional theory package, by the characterization of topological semimetals. It enables the calculation of the chirality (or “monopole charge”) associated with band crossings (Weyl nodes) and nodal lines. The theoretical methodology for the calculation of the chirality is based on an extended Wilson loop method and a Berry phase approach. We validated the code using TaAs, which is a well-characterized Weyl semimetal, both theoretically and experimentally. Then, we applied the method to the characterization of YRh6Ge4 and found two sets of Weyl points (ca. 0.2 eV below the Fermi energy) together with a topological nodal line (protected by mirror symmetry) crossing the Fermi energy and mapped their chiralities.

P29

Identifying Signatures of Emergent QuantumPhenomena in Bulk SrSi2using Berry PhaseCurvature and Fermi Level Topologies

We present a study on the topological and geometrical properties of strontium disilicide (SrSi2), which is a Weyl semimetal in the ground state without spin-orbit coupling. The evolution of the electronic band structure of the crystal as a function of external perturbations such as strain, electric field and magnetic field, and in the presence of spin-orbit coupling, exhibits new and interesting features that require further investigation.

P30

Crystal Hall effect and effect of bi-axial strain in the anomalous Hall effect of $SrRuO_3$ thin-films

Abstract:
Motivated by the recently observed topological Hall effect in ultrathin films of $SrRuO_3$(SRO) grown on $SrTiO_3$(STO) substrate, we investigate the effect of strain-induced oxygen octahedral distortion in the electronic structure, magnetic ground state and anomalous Hall response of the SRO ultra-thin films by virtue of density functional theory calculations. In the mono-layer limit, large energy level splitting of Ru-t_{2g} states, caused by compressive strain in the thin film layer, stabilizes an anti-ferromagnetic (AFM) insulating magnetic ground state. From the systematic investigation of our results, the large Hall effect in compensated antiferromagnets is identified as a clear manifestation of the so-called crystal Hall. For Ferromagnetic SRO films (tri-layer of SRO), we find a strong deformation of the oxygen octahedral (RuO6) with an increasing amount of substrate induced compressive strain. Our Berry curvature calculations predict a positive value of the anomalous Hall conductivity of +76 S/cm at -1.7% strain, whereas it is found to be negative (-156 S/cm) at -0.47% strain. We attribute the observed behaviour of the anomalous Hall effect to the nodal point dynamics in the electronic structure arising in response to tailoring the oxygen octahedral distortion driven by the substrate induced strain.

P31

Hidden interplay of current-induced spin and orbital torques in bulk Fe3GeTe2

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Low crystal symmetry of magnetic van der Waals materials naturally promotes spin-orbital complexity unachievable in common magnetic materials used for spin-orbit torque switching. The van de Waals ferromagnet Fe_3GeTe_2 (FGT), has already proved highly efficient at this particular mechanism [1], yet rich skyrmionic textures [2] and semi-metallicity [3] are also found within its roster of ever-growing phenomena. In a recent collaboration [4] we found that spin-orbit torques (SOTs) were observed within the bulk, yet the clean crystal's bilayer system is centrosymmetric. Recent evidence has given light to a site preference that breaks this symmetry [5], implying bulk SOTs are possible. To understand their origin, however, one must delve into the layer resolved components to provide a comprehensive understanding of the current-induced response of its complex electronic structure.

Here, using first-principles methods [6], we demonstrate that whilst the clean system leads to overall vanishing spin-orbit torques, strong 'hidden' current-induced torques are harvested by each of the two-dimensional FGT layers separately. Such strong layer-dependent torkances can then be unlocked by its aforementioned site preference. Analysis of the electronic structure elucidates an interplay of spin and orbital degrees of freedom which have a profound impact on spin-orbit torques. A drastic difference in the behaviour of the individual components of the torque result in a non-trivial switching. Our findings promote the design of the non-equilibrium orbital response as the guiding mechanism for crafting the properties of spin-orbit torques in layered van der Waals materials.

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P32

Electronically driven anharmonicity in charge-density-wave materials

Charge-density waves (CDWs) occupy an important position in the phase diagram of low-dimensional systems such as the transition metal dichalcogenide monolayers. Although a CDW can often be identified already from the undistorted structure in linear response, anharmonic effects are eventually responsible for the stabilization of the distorted phase and its precise properties. To study the mechanisms responsible for the anharmonicity, we calculate Born-Oppenheimer potential energy surfaces for lattice distortions in 1T-TaS2, 1T-VS2, and 2H-TaS2, and we establish a connection to the electronic structure of these materials.

P33

Using TD-MLWFs to Study Electronic Excitations in Exascale Systems with Massively Parallel Real-Time TDDFT

We discuss how propagating time-dependent maximally-localized Wannier functions (TD-MLWFs) can provide key insights at the molecular level when studying electronic excitation and dynamics in complex, exascale systems, using real-time time-dependent density functional theory (RT-TDDFT). In particular, our implementation in the massively parallel Qb@ll code is discussed, and we present its application to studying non-equilibrium energy transfer excitation in solvated DNA under ion irradiation. We further discuss how hybrid DFT functionals can be implemented efficiently using the time-dependent MLWFs.

P34

Gate tunable anomalous Hall effect at (111) LaAlO 3 /SrTiO 3 inteface

The Rashba interaction couples the electron spin momentum with its orbital motion allowing for spin-charge conversion tunable via electric field in 2D materials and gives rise to many interesting phenomena, like anomalous Hall effect [1]. Transition metal oxides, characterized by a strong spin- orbit coupling, are suitable materials to exploit such a phenomenon [2]. Here we develop a tight- binding model for electronic band structure of the (111) LaAlO 3 /SrTiO 3 heterostructure interface, and derive a generalized Rashba coupling in terms of the total angular momentum J near the bottom of the bands. Moreover, breaking the time-reversal invariance, i.e. using a magnetic field, induces a non-vanishing Berry Curvature with multiband character that causes anomalous Hall phenomena when an in-plane electric field is added. The anomalous Hall conductivity shows a peculiar dependence on the fillings which can be understood on the basis of our J model.

P35

Doping induced ferromagnetism in $EuTiO_3$ and STO/ETO/LAO heterostructures by ab-initio calculations

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The emergence of a quasi two-dimensional electron gas (2DEG) at the interface of two metal oxides as $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) raised an immense interest in the community of oxide electronics, insofar as this system was found to be blessed with a plethora of outstanding properties such as field-effect driven superconductivity, high electron mobility and magnetoresistance. An old dream of the spintronic community, remained substantially eluded so far, has been the possibility to inject magnetization in the 2DEG by introducing a magnetic layer at the interface of LAO/STO heterostructure. This may create spin-polarized 2DEG, and enable this system as a paramount material for spintronics and spin-orbitronic technology. A serious candidate as magnetic interlayer is $EuTiO_3$ (ETO), proposed in recent years by experiments [1]. ETO has cubic perovskite crystal structure and has nearly identical lattice constant to STO. It is reported that bulk ETO has G-type AFM ground state below $T_n = 5.3$ K, while it becomes FM under tensile strain or doping [2, 3]. We have applied several ab-initio approaches (GGA, GGA+U, and HSE06 functionals) to study structural, electronic and magnetic properties of ETO bulk and the STO/ETO/LAO heterostructure. We found, for increasing electron doping, a progressive enhancement of the FM phase stability under doping. We also applied the Wannier function interpolation to explore the magnetic interactions in ETO. Our results show that Eu-Ti-Eu coupling is predominant over direct Eu-Eu coupling, while intra-Eu $4f$-$5d$ virtual excitations are fundamental to drive FM coupling under n-doping. In fact, for increasing electron doping, the whole charge entirely goes to fill majority Ti-$3d$ t_{2g} orbitals, while a small but significant residual magnetization $\sim$0.05 μB is also present, even at zero doping, on the Eu-$5d$ states, indicating strong $4f$-$5d$ hybridization. Overall, our results for n-doped ETO and STO/ETO/LAO heterostructures depict them to be potential candidates for electronic transport and magneto-transport applications.

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