MM 12: Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Monday 15:45–17:45 H51

Talk MM 12.1 Mon 15:45 H51

Mechanism of Li intercalation/deintercalation into/from the surface of $LiCoO_2$ — •Ashkan Moradabadi and Payam Kaghazchi — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

$LiCoO_2$ is the most commonly used cathode material in Li-ion batteries. In this work, we have investigated atomic and electronic structures, magnetic properties, formation energies, and energy barriers for the diffusion of Li in single vacancies, divacancies, and missing rows in bulk and surface of $LiCoO_2$. Our GGA-PBE results indicate that there is almost no energy barrier for the Li-ion deintercalation from the surface layer. Energy barrier for the Li-ion intercalation is also very small. However, we find that Li hopping in PBE+U is accompanied by electron hopping between nearby transition metal ions. Therefore a PBE+U barrier, which is for both Li hopping and charge hopping, is higher than the corresponding PBE barrier [1]. This study has implications in understanding the role of the surface in the rate capability of nanostructured $LiCoO_2$ cathodes of Li-ion batteries.

[1] Ashkan Moradabadi and Payam Kaghazchi, Mechanism of Li intercalation/deintercalation into/from the surface of $LiCoO_2$, Phys. Chem. Chem. Phys., 2015, 17, 22917-22922.

Talk MM 12.2 Mon 16:00 H51

Potential-dependent mechanism of Li diffusion in Li_2S — •Ashkan Moradabadi[1,2] and Payam Kaghazchi[1] — [1]Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany — [2]Institut für Materialwissenschaft, Fachgebiet Materialmodellierung, Technische Universitat Darmstadt, Jovanka-Bontschits-Str. 2, 64287 Darmstadt, Germany

Li-S batteries are promising candidates for large-scale applications such as electrical vehicles. However, the measured discharge capacity is often less than the theoretical one [1,2]. This is mainly due to the slow diffusion of Li through Li_2S shells formed on S_8 cores, which leads to an incomplete conversion of S_8 cores to Li_2S (the final product of lithiation of S_8). In the present work, using density functional calculation, we have investigated mechanism of Li diffusion in Li_2S. At low cell voltages (¡ 0.93 V), Li diffusion occurs via an exchange mechanism with a high energy barrier of 0.45 eV. However at higher cell voltages, Li diffusion takes place via a vacancy mechanism with a lower energy barrier of 0.27 eV. Our findings can explain the capacity fading in Li-S batteries at high operation rates.

[1] Liang, X.; Hart, C.; Pang, Q.; Garsuch, A.; Weiss, T.; Nazar, L. F.; A highly efficient polysulfide mediator for lithium-sulfur batteries. Nature Communications, 2015, 6, 5682.

[2] Wang, L.; Wang, Y.; Xia, Y.; A high performance lithium-ion sulfur battery based on a Li_2S cathode using a dual-phase electrolyte. Energy Environ. Sci. 2015, 8, 1551.

Talk MM 12.3 Mon 16:15 H51

Extremely high magnetoresistance in topological insulator candidate LaBi — •Nitesh Kumar, Chandra Shekhar, and Claudia Felser — Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany.

Lanthanum monopnictides (LaX, X=N, P, As, Sb, Bi) have recently been predicted to be topological insulators, except LaN which is a topological semimetal. Inspired from this report we have studied the transport properties of LaBi. It has a simple rock salt-type structure with alternate La and Bi atoms arranged in all three directions. Temperature variation of resistivity at different magnetic fields follows Kohler's rule. Resistivity follows almost a parabolic relation with magnetic field without saturation, exhibiting a huge magnetoresistance (1.5 x10^5% at 2 K and 9 T). By employing two band model we calculate carrier density and mobility of electrons and holes which suggests that LaBi is a compensated system. We believe this to be responsible for high unsaturated MR in LaBi. We observe excellent Shubnikov-de Haas (SdH) oscillations starting from around 3T. We also analyse the angle and temperature dependence of these oscillations.

Talk MM 12.4 Mon 16:30 H51

VOTCA-STP - Multi Scale Modeling of Spin Transport in Organic Semiconductors — •Erik R. McNellis, Shayan Hematiyan, Amaury Melo Souza, Sebastian Müller, and Jairo Sinova — Johannes Gutenberg University, Mainz, Germany

Organic molecules present a range of unique and highly attractive properties in solid state technology applications. So also in spintronics, where the weak but highly tailorable spin-orbit coupling in light elements offers spin lifetimes of unparalleled length and controllability.

1st-principles theoretical modeling stands to provide a crucial perspective on the emerging field of spin transport in organic semiconductors. Comprehensive modeling of relevant systems is challenging, with several of the spin transport mechanisms in traditional solid state materials non-existent or strongly modified in organics.

We are developing a multi-scale modeling framework for spin transport in bulk organic materials, based on the VOTCA toolkit for charge transport in the same. The core component is a semi-classical kinetic Monte-Carlo model, with input parameters calculated using 1st-principles theory.

The scope, capabilities of and particular challenges for this development will be presented along with possible extensions to e.g. 'spinterfaces', where spin currents are manipulated by tailoring of an inorganic / organic solid interface, as well as a perspective on the potential ramifications for experimental work in the field.

15 min. coffee break

Talk MM 12.5 Mon 17:00 H51

High-pressure and nonlinear elastic response of solids: Example of carbon allotropes — •Pasquale Pavone, Rostam Golesorkhtabar, Stefan Kontur, and Claudia Draxl — Humboldt-Universität zu Berlin, Physics Department and IRIS Adlershof, 12489 Berlin, Germany

As prototype materials showing strong nonlinear elastic behaviour, diamond and, more recently, layered carbon allotropes have attracted much attention. However, even the nonlinear elasticity of diamond is not completely clarified: Experimentally, nonlinear elastic constants of diamond were investigated only recently [1], showing significant discrepancies with theoretical results. Furthermore, the standard ab-initio reference calculation for diamond [2] is nowadays about 30 years old and needs to be updated in the light of current development of theory, numerical algorithms, and available computer power. Using the full-potential all-electron package `exciting` [3], we perform a systematic ab-initio investigation of the nonlinear elastic properties of diamond, graphene monolayers, as well as simple-hexagonal and hexagonal graphite. We develope an extension of the `ElaStic` tool [4] for the determination of third-order elastic constants. From these results the pressure dependence of linear elastic constants is obtained and connected to dynamical quantities like the mode Grüneisen parameters.

[1] J.M. Lang *et al.*, Phys. Rev. Lett. **106**, 125502 (2011).
[2] O.H. Nielsen, Phys. Rev. B **34**, 5808 (1986).
[3] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[4] R. Golesorkhtabar *et al.*, Comp. Phys. Commun. **184**, 1861 (2013).

Talk MM 12.6 Mon 17:15 H51

Calculations of temperature dependent resistivity for transition metals from the first principles — •David Wagenknecht[1,2], Ilja Turek[1,2], and Karel Carva[1] — [1]Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University in Prague; Ke Karlovu 3, 12116 Prague 2, Czech Republic — [2]Institute of Physics of Materials, Academy of Sciences of the Czech Republic; Žižkova 22, 61662 Brno, Czech Republic

The temperature dependence of electrical resistivity is studied from the first principles. Properties of late transition metals have been calculated using the linear muffin-tin orbital (LMTO) method with the coherent potential approximation (CPA). The influence of non-zero temperature has been described by a frozen lattice disorder – atoms were moved from the positions on an ideal lattice and different temperatures are then given by the magnitudes of the random displacement vectors. Dependence of the physical quantities on the parameters of the displacements (like random and non-random directions of the displacement vectors) has been observed and taken into account during discussion of the results. Special attention has been paid to an influence of spin-orbit interaction on the final resistivity, as well as to comparison with other *ab initio* calculations and experimental data; the obtained results agree reasonably well with those of other authors. Derived analytical modifications of the LMTO potential functions and the numerical codes can be now used to calculate relevant physical properties of different materials.

Talk MM 12.7 Mon 17:30 H51

Ab Initio Molecular Dynamics Study of Conjugated Polymer Systems: The Elusive Localization of the Polaron — •Håkan W. Hugosson[1], Amina Mirsakiyeva[1], and Anna Delin[1,2] — [1]Department of Materials och Nano Physics, KTH Royal Institute of Technology, Stockholm, Sweden. — [2]Ångstrom Laboratory, Uppsala University, Uppsala, Sweden.

The thermoelectric conjugated polymer poly(3,4-ethylenedioxythiophene), or PEDOT, contains a carbon backbone consisting of alternating short and long carbon bonds. Therefore there are two isomeric states: aromatic and quinoid. Charge injection or the presence of charged doping agents leads to the formation of localized charge in the conjugated polymer - a so-called polaron. This polaron induces a localized structural distortion (a shift from the aromatic form towards the quinoid) in the conjugated carbon backbone.

Self-localized polarons in conjugated carbon systems have been found using semi-empirical or HF-theory, but formerly never using DFT with local or gradient corrected functionals (e.g. LDA/BLYP). Self-localization has been seen using DFT and long range hybrid functionals with partial exact exchange included.

Using modern ab initio molecular dynamics methods based on DFT we have studied PEDOT and its charge carrying polarons. A localized polaron is now found when studying the time-averaged changes in bond-distances and also in snap-shots for the frontier orbitals for long oligomers (12 monomers).

O 41: Frontiers of Electronic Structure Theory: Focus on Topology and Transport I

Tuesday 14:00–16:00 H24

Topical Talk O 41.1 Tue 14:00 H24

Topological semimetals and chiral transport in inversion asymmetric systems — •Shuichi Murakami — Department of Physics and TIES, Tokyo Institute of Technology, Tokyo, Japan

Weyl semimetals (WS) are semimetals with nondegenerate 3D Dirac cones in the bulk. We showed that in a transition between different Z2 topological phases, the Weyl semimetal phase necessarily appears when inversion symmetry is broken. In the presentation we show that this scenario holds for materials with any space groups without inversion symmetry. Namely, if the gap of an inversion-asymmetric system is closed by a change of an external parameter, the system runs either into (i) a Weyl semimetal phase or (ii) a nodal-line semimetal, but no insulator-to-insulator transition happens. This transition is realized for example in tellurium (Te). Tellurium has a unique lattice structure, consisting of helical chains, and therefore lacks inversion and mirror symmetries. At high pressure the band gap of Te decreases and finally it runs into a Weyl semimetal phase, as confirmed by our ab initio calculation. We also theoretically propose chiral transport in systems with such helical structures.

Talk O 41.2 Tue 14:30 H24

Topological orbital magnetic moments — •Manuel dos Santos Dias, Juba Bouaziz, Mohammed Bouhassoune, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Orbital magnetic moments are usually associated with the spin-orbit interaction (SOI). We explore from first-principles how topological orbital magnetic moments (TOMs) can emerge in non-trivial magnetic spin textures, even without SOI, justifying the 'topological' label. Firstly, the case of magnetic trimers on the Cu(111) surface illustrates the basic symmetry properties of the TOMs, and how to separate their contribution from the usual SOI-driven orbital moments. We then focus on the implications of TOMs for single magnetic skyrmions formed in Pd/Fe/Ir(111) [1], considering their possible use in detecting and distinguishing skyrmions from anti-skyrmions by optical means.

Work funded by the HGF-YIG Programme FunSiLab – Functional Nanoscale Structure Probe and Simulation Laboratory (VH-NG-717).

[1] D.M. Crum et al., Nat. Comms. **6**, 8541 (2015)

Talk O 41.3 Tue 14:45 H24

The orbital Rashba effect — •Dongwook Go[1,2], Patrick Buhl[1], Gustav Bihlmayer[1], Yuriy Mokrousov[1], Hyun-Woo Lee[2], and Stefan Blügel[1] — [1]Institute for Advanced Simulation and Peter Grünberg Institut, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Department of Physics, Pohang University of Science and Technology, 37673 Pohang, Korea

We present a new surface phenomenon called the *orbital* Rashba effect, analogous to the spin Rashba effect. The effect is described by the orbital Rashba Hamiltonian, $H_{\text{orb-R}}(\mathbf{k}) = \alpha_{\text{orb-R}}\mathbf{L}\cdot(\hat{\mathbf{z}}\times\mathbf{k})$, where $\mathbf{L}$ is the orbital moment derived from atomic orbitals and $\alpha_{\text{orb-R}}$ is the orbital Rashba constant. This leads to orbital-dependent energy splittings and orbital texture in the $\mathbf{k}$-space. The mechanism behind the emergence of the $H_{\text{orb-R}}(\mathbf{k})$ can be understood as the $\mathbf{k}$-dependent magnetoelectric coupling due to atomic orbital hybridization. In the presence of intra-atomic spin-orbit coupling, the spin moment is aligned parallel or antiparallel to the orbital moment, thus the spin Rashba effect is recovered. As an example, we present a tight-binding and an *ab initio* study of the Bi/Ag(111) surface alloy, where the hybridization between a Ag *s*-orbital and a Bi *p*-orbital leads to the orbital Rasbha effect that is dominant over the spin one. The orbital Rashba effect is a key to new physics and to understanding spin-orbit driven physics at surfaces and interfaces, such as Dzyaloshinskii-Moriya interaction, non-collinear magnetism, etc.

Talk O 41.4 Tue 15:00 H24

Spin and orbital magnetism of Rashba electrons induced by magnetic nanostructures — •Juba Bouaziz, Manuel dos Santos Dias, Phivos Mavropoulos, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We explore theoretically the spin and orbital magnetism of Rashba electrons in the presence of noncollinear impurity-induced magnetic states. The Rashba electron gas mediates the Dzyaloshinksii-Moriya interaction between magnetic impurities favoring chiral states [1]. Here we investigate the back-action of such noncollinear magnetic states on the Rashba electron gas. The presence and distribution of ground state spin and orbital currents is analyzed. Surprisingly, when switching off the spin-orbit coupling, chiral magnetic textures generate bound currents, which implies the existence of orbital magnetic moments originating solely from the peculiar topology of the impurities magnetic moments. In the particular case of a single adatom with an out of plane magnetic moment, we found circular currents flowing around the magnetic impurity in agreement with the continuity equation for the electric charge. Similar results were predicted for magnetic adatoms on superconductor surfaces with a finite spin-orbit coupling [2].

[1] J. Bouaziz *et al.* in preparation.
[2] S. S. Pershoguba *et al.* Phys. Rev. Lett. **115**, 116602 (2015).

This work is supported by the HGF-YIG Programme VH-NG-717 (Functional Nanoscale Structure and Probe Simulation Laboratory).

Talk O 41.5 Tue 15:15 H24

First-principles investigation of the impact of single atomic defects on magnetic skyrmions — •Imara L. Fernandes, Benedikt Schweflinghaus, Juba Bouaziz, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

Chiral magnetic skyrmions are topological spin-swirling textures with rich physics and technological potential in the field of information storage. In a device, skyrmions certainly interact with defects and imperfections resulting into pinning phenomena. We explore from first-principles the non-trivial impact of 3d and 4d impurities on the energetics, electronic and magnetic properties of single magnetic skyrmions. Utilizing the newly developed Jülich full-potential relativistic Korringa-Kohn-Rostoker Green function method [1], we focus on topological magnetic objects of sub-5nm diameters stabilized in a single ferromagnetic layer of Fe sandwiched between the Ir(111) surface and one or two Pd layers, where the tunneling spin-mixing magnetoresistance (TXMR) was demonstrated theoretically [2] and experimentally [3]. – Funding provided by the HGF-YIG Program VH-NG-717 and the CNPq (BRAZIL).

[1] D. S. G. Bauer, Schriften des Forschungszentrum, Key Tech. **79**

(2014).
[2] D.M. Crum *et al.*, Nat. Comms. **6**, 8541 (2015).
[3] C. Hanneken *et al.*, Nat. Nanotech. Doi:10.1038/nano.2015.218 (2015).

Talk O 41.6 Tue 15:30 H24

Topological magnons: Any chance to find them? — •Alexander Mook[1], Jürgen Henk[2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, D-06120 Halle — [2]Institut für Physik, Martin-Luther-Universität, D-06120 Halle

Topological magnon insulators (TMIs) have a nontrivial topology due to the Dzyaloshinskii-Moriya interaction which results in spatially confined edge states and, thus, energy and spin currents along their edges [1,2]. Several systems have been identified as TMIs, for example, Cu(1,3-benzenedicarboxylate) consisting of kagome planes [3], or the family of ferromagnetic pyrochlore oxides, e. g., $Lu_2V_2O_7$, showing the magnon Hall effect [4]. However, to date, no direct experimental evidence of a topological magnon band has been provided, what comes down to the small total width of the magnon dispersion relation and the energy resolution of surface sensitive measurements.

We propose Fe_3Sn_2 as promising candidate for a TMI. The total width of its magnon dispersion relation is large, and we determine its nontrivial topology by constructing an effective spin Hamiltonian. On this basis, we discuss signatures of topological magnon states that should be looked for in experiments.

[1] L. Zhang et al., PRB **87**, 144101 (2013); [2] A. Mook et al., Phys. Rev. B **89**, 134409 (2014); *eidem*, Phys. Rev. B **90**, 024412 (2014); *eidem*, Phys. Rev. B **91**, 224411 (2015); *eidem*, Phys. Rev. B **91**, 174409 (2015); [3] R. Chisnell et al., Phys. Rev. Lett. **115**, 147201 (2015); [4] Y. Onose et al., Science **329**, 297 (2010).

Talk O 41.7 Tue 15:45 H24

Acoustic magnons in the long-wavelength limit: resolving the Goldstone violation in many-body perturbation theory — •Mathias C.T.D. Müller, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Ferromagnetic materials exhibit a spontaneously broken global rotation symmetry in spin space leading to the appearance of massless quasiparticles (zero gap) in the long-wavelength limit. These magnons are formed by the correlated motion of electron-hole pairs with opposite spins, which we describe from first principles employing the T-matrix formalism in the ladder approximation within the FLAPW method [1]. Due to approximations used in the numerical scheme, the acoustic magnon dispersion exhibits a small but finite gap at Γ. We analyze this violation of the Goldstone mode and present an approach that implements the magnetic susceptibility using a renormalized Green function instead of the Kohn-Sham (KS) one. This much more expensive approach shows substantial improvement of the Goldstone-mode condition. In addition, we discuss a possible correction scheme, that involves an adjustment of the KS exchange splitting, which is motivated by the spin-wave solution of the one-band Hubbard model. The new exchange splittings turn out to be closer to experiment. We present corrected magnon spectra for the elementary ferromagnets Fe, Co, and Ni.

[1] E. Şaşıoğlu *et al.*, Phys. Rev. B **81**, 054434 (2010); C. Friedrich *et al.* Top. Curr. Chem. **347**, 259 (2014).

O 55: Frontiers of Electronic Structure Theory: Focus on Topology and Transport II

Wednesday 10:30–13:00 H24

Talk O 55.1 Wed 10:30 H24

Coupled-Cluster approach for both molecules and solids in the numeric atom-center orbital framework — •Tonghao Shen, Arvid Conrad Ihrig, Igor Ying Zhang, and Matthias Scheffler — *Fritz-Haber-Institut der MPG, Berlin.*

For a quantitative prediction of material properties, an advanced description of electronic correlation is crucial. As the "gold standard" correlation method in quantum chemistry, the coupled-cluster (CC) ansatz with singles, doubles and perturbative triples (CCSD(T)) is starting to gain attention in materials science[1]. At present, the CCSD(T)-quality description of the correlation effects in solids can be achieved by either studying the cluster-size convergence toward the bulk in real space[1] or implementing CCSD(T) for extended systems in reciprocal space[2]. In order to investigate and compare these approaches on an equal footing, it is essential to have a computational platform that enables CCSD(T) simulations to be carried out using both cluster and periodic models in a single computational environment. In this report, we present a CCSD(T) implementation for both molecules and solids in the all-electron full-potential code FHI-aims[3] with numeric atom-center orbital(NAO) basis sets. A special memory-distribution strategy is designed to significantly reduce the inter-CPU communication, which is the main challenge for the parallelization of wave-function methods. The accuracy and efficiency are demonstrated for a group of molecules, 1D-, 2D- and 3D-periodic materials. [1] C. Müller, *et al.*, PCCP. **14**, 7605 (2012); [2] A. Grüneis, *et al.*, JCTC **7**, 2780 (2011); [3] V. Blum, *et al.*, CPC **180**, 2175-2196 (2009).

Talk O 55.2 Wed 10:45 H24

Surface adsorption energetics at the "gold standard": Small molecule binding to TiO_2(110) — •Daniel Berger[1,2], A. Kubas[3], D. Manganas[3], H. Oberhofer[1], F. Neese[3], and K. Reuter[1] — [1]TU München — [2]University of California, Los Angeles — [3]MPI für chemische Energiekonversion, Mülheim an der Ruhr

Adsorption energies at oxide surfaces are central quantities required for catalysis, energy and a multitude of other application areas. At present, the by far dominant computational method to obtain such energetics is density-functional theory (DFT). Unfortunately, systematic benchmarking of such energetics against accurate reference numbers from correlated wave-function theory as known from molecular systems is scarce, largely owing to the fact that the latter techniques are often not available for standard periodic boundary condition supercell calculations.

We address this situation with a solid-state QM/MM embedded cluster approach, in which the adsorbate and immediate surrounding surface atoms are described quantum mechanically, while the long-range electrostatic interactions are accounted for through a polarizable force field. This yields a numerically highly efficient approach that enables use of the recently developed domain-based local pair natural orbital coupled cluster method with single-, double- and perturbative triple-excitations (DLPNO-CCSD(T)) in the quantum region. We exploit corresponding "gold standard" adsorption energies for a set of prototypical small molecules interacting with the rutile TiO_2(110) surface for a systematic benchmark of DFT numbers.

Talk O 55.3 Wed 11:00 H24

Water adsortpion on surfaces form many-body perturbation theory — •Theodoros Tsatsoulis and Andreas Grüneis — Max-Planck-Institute for Solid State Research, Stuttgart

The accurate description of the interaction of molecules with surfaces is of crucial importance for a wide range of phenomena. While Kohn-Sham density functional theory is one of the most widely-used methods for describing the electronic structure of surfaces, many local and semi-local functionals are often not able to produce accurate molecular adsorption energies. Quantum chemical wave-function based methods such as Møller-Plesset perturbation theory (MP2) and coupled-cluster methods promise controllable accuracy, however, at much higher computational costs. Large part of the latter is due to the number of virtual states. We consider an approach whereby the occupied orbitals are converged in a plane wave basis, whereas the virtual space is then constructed using pseudized Gaussian orbitals expanded in plane waves, leading to reduced computational cost. In particular we study water adsorption on bulk LiH and h-BN sheets at the level of MP2 theory within the projector-augmented-wave method as implemented in VASP [1]. The results are compared to state-of-the-art methods such as hybrid functionals and diffusion Monte Carlo [2].

[1] Marsman et al., The Journal of Chemical Physics, 130, 184103 (2009)
[2] Al-Hamdani et al., The Journal of Chemical Physics, 142, 181101 (2015)

Talk O 55.4 Wed 11:15 H24

Photo-isomerization in azobenzene-functionalized self-assembled monolayers: The impact of many-body effects — •Caterina Cocchi and Claudia Draxl — Institut für Physik und

IRIS Adlershof, Humboldt-Universität zu Berlin, Berlin, Germany

Self-assembled monolayers (SAMs) of azobenzene-functionalized alkanethiols on gold suffer from hindered photo-isomerization, as observed experimentally [1]. While this behavior is generally ascribed to strong intermolecular coupling, a clear microscopic understanding of this phenomenon is still missing. In order to address this question, we perform a first-principles study of the excited-state properties of azobenzene-functionalized SAMs. In the framework of many-body perturbation theory (GW approximation and Bethe-Salpeter equation), as implemented in the all-electron full-potential code exciting [2], we investigate the optical absorption spectra of these materials, inspecting the influence of packing density and functionalization of the azobenzene molecules with different end groups. Through a systematic analysis of the character of the excitations, we clarify the role and interplay of screening and local-field effects, which strongly impact light absorption and hence photo-isomerization in these systems.

[1] C. Gahl et al. J. Am. Chem. Soc. 132, 1838 (2010). [2] A. Gulans et al. J. Phys.: Condens. Matter 26, 363202 (2014).

Talk O 55.5 Wed 11:30 H24

Laplace-transformed MP2 with localized Resolution of Identity -efficient in-memory MP2 for large systems — •Arvid Conrad Ihrig[1], Patrick Rinke[2], Igor Ying Zhang[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Aalto University, Helsinki, Finland

A well-known problem in local and semi-local density functional approximations and to a lesser extend also in hybrid functionals is the one-electron self-interaction error, which can lead to a qualitatively wrong description for applications like charge-transfer systems. One possible remedy is the 2nd order Møller-Plesset perturbation theory (MP2), which does not suffer from this error. However, the time and memory requirements for MP2 prevent it routine-use for large molecular and periodic systems. The Laplace-transformed MP2 (LT-MP2) [1] can significantly reduce the computational time, but requires the usage of intermediate variables stored on disk, resulting in an inefficient usage of computational resources. In this work we combine the LT-MP2 with our localized Resolution of Identity (RI-LVL) [2] approach to eliminate the disk-storage bottleneck and fully exploit massive parallelization strategies. RI-LVL expands the basis function pairs in the electron repulsion integrals in local auxiliary basis sets. For the example of water clusters, we demonstrate the favourable memory scaling (at worst N^2) of our new MP2 implementation, which facilitates the in-memory calculation of large systems at high accuracies.

[1] P. Ayala et al., J. Chem. Phys. 110, 3660 (1999)
[2] Ihrig et al., New J. Phys. 17, 093020 (2015)

Talk O 55.6 Wed 11:45 H24

***GW* singles contributions for the random phase approximation correlation energies** — •Jiri Klimes[1], Merzuk Kaltak[2], Emanuele Maggio[3], and Georg Kresse[3] — [1]J. Heyrovský Institute of Physical Chemistry, Prague, Czech Republic — [2]Department of Physics and Astronomy, Stony Brook University, Stony Brook, NY — [3]University of Vienna, Faculty of Physics, Vienna, Austria

The random phase approximation (RPA) to the correlation energy yields often very accurate results for condensed matter systems. However, a general tendency to underbind has been observed for systems such as molecular solids or for adsorption. One of the ways that have been proposed to improve the accuracy of RPA are the so-called singles corrections of Ren and coworkers [1]. We present our derivation of the singles corrections using the assumption that the electron density changes when going from the reference to the interacting system [2]. This leads to a very compact expression for the corrections. Moreover, the singles formula can be easily modified to account for screening effects, giving the *GW* singles. We assess the effect of both the original and modified singles on covalently and metallically bonded systems as well as on simple weakly bonded systems. Finally, we show that adding the singles corrections leads to considerably improved adsorption energies and lattice energies of molecular solids.

[1] Ren, Tkatchenko, Rinke, Scheffler, Phys. Rev. Lett **106**, 153003 (2010).

[2] Klimeš, Kaltak, Maggio, Kresse, J. Chem. Phys. **143**, 102816 (2015).

Talk O 55.7 Wed 12:00 H24

Long-range corrected DFT meets *GW*: Vibrationally resolved photoelectron spectra from first principles — •Thomas Körzdörfer — Institut für Chemie, Universität Potsdam, D-14476 Potsdam

We introduce an entirely non-empirical and computationally efficient scheme to calculate highly reliable vibrationally resolved photoelectron spectra for molecules from first principles.[1] To this end, we combine non-empirically tuned long-range corrected hybrid functionals with non-self-consistent many-body perturbation theory in the G_0W_0 approximation and a Franck-Condon multi-mode analysis based on DFT-calculated frequencies. The vibrational analysis allows for a direct comparison of the GW-calculated spectra to gas-phase ultraviolet photoelectron measurements of neutral and anionic molecules, respectively. In addition, vertical IPs and EAs were benchmarked against other *GW* methods and basis-set extrapolated CCSD(T) results for a recently introduced test set of 24 molecules frequently used in organic electronics.[2] G_0W_0@LRC-DFT yields mean absolute errors on the order of 0.1 eV for IPs, EAs, and fundamental gaps, clearly outperforming commonly used G_0W_0 approaches as well as partially and fully self-consistent *GW* methods.

[1] L. Gallandi and T. Körzdörfer, JCTC **11**, 5391 (2015).
[2] L. Gallandi, N. Marom, P. Rinke, and T. Körzdörfer, JCTC *accepted for publication* (2015).

Talk O 55.8 Wed 12:15 H24

LDA-1/2 as a starting point for G_0W_0 calculations — •Ronaldo Rodrigues Pela[1,2], Ute Werner[1], Dmitrii Nabok[1], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik and IRIS Adlershof, Berlin, Germany — [2]Instituto Tecnológico de Aeronáutica, São José dos Campos, Brazil

For many semiconductors and insulators, LDA represents a bad starting point for G_0W_0 calculations. Hybrid functionals improve upon LDA, but at the price of increasing computational cost of about 2 orders of magnitude. An alternative starting-point for the single-shot G_0W_0 can be the LDA-1/2 method [1], because it approximately includes the self-energy of quasi-particles within a generalized Kohn-Sham scheme, leading to improved band-gaps over the LDA ones, but without being computationally more involved. In this work, we systematically compare 3 starting-points for G_0W_0 calculations: LDA, PBE0, and the LDA-1/2 method. A selection of semiconductors (C, Si, SiC, AlP, LiF, MgO, Ne, Ar, GaN, GaAs, CdS, ZnS, and ZnO) is chosen for this benchmark. We demonstrate that LDA-1/2 is a good choice in most cases, reducing the root mean square error in band-gap predictions by 50% when compared to G_0W_0 on top of LDA or PBE0. With the exception of large band gap materials, LDA-1/2 predictions are already close to the experimental band gaps, and thus G_0W_0 has minor effects.

Reference [1]: Phys. Rev. B 78, 125116 (2008).

Acknowledgements: "Coordenação de Aperfeiçoamento de Pessoal de Nível Superior" (CAPES) and "Alexander von Humboldt Stiftung".

Talk O 55.9 Wed 12:30 H24

DFT+U within a numeric atom-centered orbital basis — •Matthias Kick, Harald Oberhofer, and Karsten Reuter — Technische Universität München

Materials like transition metal oxides (TMOs) still challenge a description through first-principles density-functional theory (DFT). Appropriately capturing the electron localization in TMOs generally requires at least hybrid exchange-correlation functionals. Such higher-rung functionals come with appreciable computational cost, which limits their use in large supercell calculations. For such applications effective and numerically less intense approaches are therefore still a much sought alternative.

One such method is the DFT+U approach, where the on-site Coulomb correlation effects are treated using a model Hamiltonian, while remaining interactions are treated on the level of semi-local DFT. Full DFT+U functionality including nuclear gradients (forces) has been implemented in the electronic structure code *FHI-aims*. We account for three common occupation matrix representations, differing in the way how the occupations of the correlated subspaces are determined. We critically discuss their performance and differences in the context of the numeric atomic orbital basis sets employed in *FHI-aims*. The established numerically efficient framework is finally used to address neutral and charged oxygen vacancies at the TiO_2(110) surface within a solid-state embedding approach.

Talk O 55.10 Wed 12:45 H24

High-throughput Screening and Statistical Learning for Design of Transparent Conducting Oxides — •Christopher Sutton, Luca M. Ghiringhelli, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft

Transparent conducting oxides (TCOs) represent a class of well-

developed and commercialized wide-bandgap semiconductors that are crucial for many electronic devices. Ternary Al, Ga, and In-based sesquioxides are investigated as alternative wide-bandgap semiconductors motivated by very intriguing recent experimental work that has demonstrated bandgap engineering in (GayIn1-y)2O3 from 3.8 eV to ca. 5 eV[1] and ca. 5 eV to 7.5 eV for (Al1-xGax)2O3.[2]

New ternary oxides with the chemical structure of (AlxGayIn1-x-y)2O3 have been identified using cluster expansion (CE) models combined with fast stochastic optimization techniques (e.g., Wang-Landau and diffusive nested sampling) in order to efficiently search potential (ordered and disordered) configurations within a given lattice and for different temperatures. Wang-Landau and diffusive nested sampling has also allowed for a consideration of the effect of entropy on the relative stability of ternary oxides. Statistical learning has also been used to identify a structure-property relationship to efficiently identify new wide-band gap TCOs to improve the fundamental chemical and physical properties (e.g., conductivities, mobilities, and optical transparency) by investigating the parameters that control these properties.

[1] F Zhang, et al., Solid State Communications 2014, 186, 28. [2] H Ito, et al., Japanese Journal of Applied Physics 2012, 51, 100207.

O 62: Frontiers of Electronic Structure Theory: Focus on Topology and Transport III

Wednesday 15:00–18:30 H24

Topical Talk O 62.1 Wed 15:00 H24

Topological semimetal phases in strained HgTe-based alloys — Tomáš Rauch[1], Steven Achilles[1], •Jürgen Henk[1], and Ingrid Mertig[1,2] — [1]Martin Luther University Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Topological insulators (TIs) have matured to a class of materials that is studied worldwide with great effort. Prominent examples are HgTe, the Bi chalcogenides, and SnTe. Recently, the set of "original" TIs has been extended by topological semimetals: the topological Dirac and the Weyl semimetals, both of them showing point-like Fermi surfaces in the bulk. Weyl points appear always in pairs with opposite topological charges of ± 1; their projections onto the surface Brillouin zone are connected by a Fermi arc, i. e. a sizably spin-polarized topological surface state with an open Fermi contour.

In this presentation I report on theoretical investigations of strained $HgTe_{1-x}S_x$ alloys [1], with surprising results. ($\imath$) In the strong TI phase, the spin chirality of the topological nontrivial surface state can be reversed by moderate strain and changing the alloy concentration x. ($\imath\imath$) On top of this, we observe a Dirac and a Weyl semimetal phase. These findings call for experimental verification and extend significantly the "topological playground" for spin-dependent transport.

[1] T. Rauch, S. Achilles, JH, I. Mertig, Phys. Rev. Letters **114** (2015) 236805.

Topical Talk O 62.2 Wed 15:30 H24

Topological surface Fermi arcs and the chiral anomaly in Weyl semimetal materials — •Binghai Yan — Max Planck Institute for Chemical Physics of Solids, Dresden

Topological Weyl semimetals represent a novel state of topological quantum matter, which not only possesses Weyl fermions (massless chiral particles that can be viewed as magnetic monopoles in momentum space) in the bulk and unique Fermi arcs generated by topological surface states, but also exhibits appealing physical properties such as extremely large magnetoresistance and ultra-high carrier mobility. In this talk, I will first present our recent theoretical [1] and ARPES [2,3] study on the topological surface states of transition-metal monopnictides, NbP, NbAs, TaP and TaAs. By visualizing the surface Fermi arcs, we discovered their Fermiology evolution with spin*orbit coupling strength. Further, we found a way to manipulate the Fermi arcs by the Lifshitz transition. I will also introduce our recent progress on the magneto-transport in the search for the chiral anomaly effect[4,5]. References: [1] Y. Sun, S. C. Wu, and B. Yan, Phys. Rev. B 92, 115428 (2015). [2] L. X. Yang, et al. Nature Physics 11, 728 (2015). [3] Z. K. Liu, et al. Nature Materials DOI: 10.1038/NMAT4457 (2015). [4] C. Shekhar, et al. Nature Physics 11, 645 (2015). [5] C. Shekhar, et al. arXiv:1506.06577 (2015).

Talk O 62.4 Wed 16:15 H24

Topological surface Fermi arcs and spin-textures of the Weyl semimetals TaAs, TaP, NbAs, and NbP — •Yan Sun[1], Shu-Chun Wu[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany. — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany

Very recently the topological Weyl semimetal (WSM) was predicted in the noncentrosymmetric compounds NbP, NbAs, TaP, and TaAs and soon led to photoemission experiments to verify the presumed topological Fermi arcs (FAs)[1,2]. In this work we have performed fully ab initio calculations of these four WSMs and revealed the FAs with spin-momentum-locked spin texture[3]. On the (001) surface, the anion (P or As) terminated surfaces are found to fit photoemission measurements well. By tracing the spin polarization of the Fermi surface, one can distinguish FAs from trivial Fermi circles. By comparing their surface states, we reveal the evolution of topological Fermi arcs from the spin-degenerate Fermi circle to spin-split arcs when the SOC increases from zero to a finite value. Our work presents a comprehensive understanding of the topological surface states of WSMs, which will be helpful for spin-revolved photoemission and transport experiments.

References

[1] L. X. Yang, Z. K. Liu, Y. Sun, et. al. Nat.Phys.11,728, (2015).

[2] Z. K. Liu, L. X. Yang, Y. Sun, et.al Nat. Mater., doi:10.1038/nmat4457,(2015).

[3] Y. Sun, S. Wu, and B. Yan, Phy. Rev. B, 92, 115428, (2015).

Talk O 62.5 Wed 16:30 H24

New electron states at the Bi/InAs(111) interface — •L Nicolaï[1,2,3], K Hricovini[2,3], J-M Mariot[4], M C Richter[2,3], O Heckmann[2,3], U Djukic[2], T Balasubramanian[5], M Leandersson[5], J Sadowski[5], J Denlinger[6], I Vobornik[7], J Braun[7], H Ebert[7], and J Minár[7,8] — [1]LMU, Munich — [2]LPMS, UCP, Cergy, France — [3]DSM-IRAMIS, Spec, Cea-Saclay, France — [4]LCP-MR, UPMC Univ. Paris 06/CNRS, France — [5]MAX-lab, Lund Univ., Sweden — [6]ALS, Berkeley, USA — [7]EST, Trieste, Italy — [8]Univ. of West Bohemia, Plzeň, Czech Republic

The Bi(111) surface is a prototype system that shows Rashba-split surface states. Theoretical studies [1] predicted non-trivial topological surface states appearing on a single bi-layer of Bi(111) and a more complex behavior was suggested for a variable film thickness as a function of the layer thickness [2]. This clearly indicates that the electronic properties of thin films of this material are quite complex and far from being fully understood. Here we present combined theoretical and ARPES studies on the electronic structure of Bi(111) films grown on InAs(111). Bi grows epitaxially on this substrate and a monocrystal of very high quality is obtained after depositing several monolayers. ARPES experiments on the samples prepared show several new electronic states not reported before. The one-step model of photoemission as implemented in the SPR-KKR package [3] allows us to identify pristine Bi bulk states coexisting with InBi surface states.[1] M. Wada et al., Phys. Rev. B 83, 121310 (2011). [2] Z. Liu et al., Phys. Rev. Lett. 107, 136805 (2011). [3] J. Braun, Rep. Prog. Phys. 59, 1267-1338 (1996).

Talk O 62.6 Wed 16:45 H24

Two-dimensional topological phases and electronic spectra of topological insulator thin films from *GW* calculations — •Tobias Förster, Peter Krüger, and Michael Rohlfing — Institut für Festkörpertheorie, Westfälische Wilhelms-Universität, 48149 Münster, Germany

We have investigated topological and electronic properties of thin films of the topological insulators Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 with thicknesses from one to six quintuple layers employing the *GW* method. The quasiparticle band structures show highly improved agreement with experiments compared to DFT. In addition to a correction of the band gaps, the energetic positions and dispersions of the surface states change significantly around $\bar{\Gamma}$ [1]. The common approach of taking the diagonal elements of the self-energy Σ as quasiparticle energies and leaving the wave functions unchanged yields unphysical results which can be overcome by diagonalizing $\mathcal{H}^{\mathrm{QP}}$. The origin of the respective off-diagonal elements in $(\Sigma - V_{xc})$ will be discussed. As the wave functions are updated, the two-dimensional topological phases (quantum spin Hall or trivial) in *GW* differ from DFT for many systems. On the basis of our results, we further argue that one cannot unambiguously

conclude the topological phase from fits to ARPES band structures as performed in recent experimental studies.

[1] T. Förster, P. Krüger, and M. Rohlfing, Phys. Rev. B **92**, 201404(R) (2015)

Talk O 62.7 Wed 17:00 H24

Steady-State Density Functional Theory for Finite Bias Conductances — •Stefan Kurth[1,2] and Gianluca Stefanucci[3,4] — [1]Dept. of Materials Physics, Univ. of the Basque Country UPV/EHU, San Sebastian, Spain — [2]IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — [3]Dept. of Physics, Univ. of Rome "Tor Vergata", Rome, Italy — [4]INFN, Frascati, Italy

In the framework of density functional theory a formalism to describe electronic transport in the steady state is proposed which uses the density on the junction and the steady current as basic variables. In a finite window around zero bias, a one-to-one map is established between the basic variables and both local potential on as well as bias across the junction. The resulting Kohn-Sham system features two exchange-correlation (xc) potentials, a local xc potential and an xc contribution to the bias. For weakly coupled junctions the xc potentials exhibit steps in the density-current plane which are shown to be crucial to describe the Coulomb blockade diamonds. At small currents these steps emerge as the equilibrium xc discontinuity bifurcates. The formalism is applied to a model benzene junction, finding perfect agreement with the orthodox theory of Coulomb blockade.

Talk O 62.8 Wed 17:15 H24

Revealing the intra-molecular origin of inelastic electron tunneling signal by means of first-principles calculations — •Giuseppe Foti and Hector Vazquez — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnicka 10, Prague, Czech Republic

We explore the intra-molecular contributions to the peaks in the Inelastic Electron Tunneling Spectrum (IETS) of a benzene-based molecular junction by means of DFT-NEGF simulations [1,2]. These contributions are calculated from the bracket of the left- and right- transmission channels with the e-ph coupling matrix by grouping the products into one- and two-atom terms. This combines the geometrical information of the vibrational modes with the electronic properties of the scattering states. Our calculations show how the partial contributions of each atom and bond in the molecule combine to give the total inelastic signal. We find that, for most of the high intensity peaks, these terms sum up constructively while dark modes result from cancellations. We also investigate the relation between the symmetry of the vibrational modes and the cancellation pattern of the different contributions. This analysis enables a real space representation of the intra-molecular contributions associated to each vibrational mode and allows a complete mapping and characterization of the origin of the IETS peaks.

[1] J. M. Soler et al. J. Phys.: Condens. Matter 14, 2745 (2002)
[2] T. Frederiksen et al. Phys. Rev. B 75, 205413 (2007)

Talk O 62.9 Wed 17:30 H24

An efficient real-time time-dependent density functional theory method and its applications — •Zhi Wang[1], Shu-Shen Li[2], and Lin-Wang Wang[3] — [1]Institut für Physikalische Chemie, Uni-Hamburg, Hamburg, Germany — [2]Institute of Semiconductors, Chinese Academy of Sciences, Beijing, China — [3]Lawrence Berkeley National Laboratory, Berkeley, United States

We have developed an efficient real-time time-dependent density functional theory (TDDFT) method that can increase the effective time step from <1 as in traditional methods to ~0.1 fs. With this algorithm, the TDDFT simulation can have comparable speed to the Born-Oppenheimer (BO) ab initio molecular dynamics (MD). The application of the method will be illustrated for several non-equilibrium systems, e.g., energetic particle colliding onto a TMDC monolayer, and ultrafast charge seperations in photovoltaic systems.

Talk O 62.10 Wed 17:45 H24

Nonadiabatic geometric phase of a pseudorotating triatomic molecule — •Ryan Requist and Eberhard K. U. Gross — Max Planck Institute of Microstructure Physics, Halle (Saale), Germany

The geometric phase of a real-valued Born-Oppenheimer electronic wavefunction is a topological quantity depending on the winding number of the path around a conical intersection of the adiabatic potential energy surfaces in nuclear coordinate space. We report the calculation of a nonadiabatic molecular geometric phase that takes the full quantum mechanical motion of the nuclei into account through the exact factorization scheme [1]. Nonadiabatic contributions "smear out" the point-like adiabatic Berry curvature, changing the topological invariant into a genuine path-dependent geometric phase [2].

[1] S. K. Min, A. Abedi, K. S. Kim and E. K. U. Gross, Phys. Rev. Lett. 113, 263004 (2014). [2] R. Requist and E. K. U. Gross, arxiv:1506.09193.

Talk O 62.11 Wed 18:00 H24

Theoretical investigations of magnetically doped topological insulators — •Jan Minar[1,2], Jurgen Braun[1], and Hubert Ebert[1] — [1]LMU München, Germany — [2]University of West Bohemia, Plzen, Czech Rep.

Band gap opening of topological surface states due to magnetic doping are the subject of a long standing discussion. However, in spite of the progress made during the last years in this field there are still phenomena that are poorly understood and many open issues to be addressed. In several cases, like for example Mn doped Bi_2Se_3 band gap opening does not seem to be of magnetic origin. Here we will present several examples detailed theoretical studies on various bulk as well as surface doped topological insulators by means of the SPR-KKR band structure method. Our results will be discussed in a direct comparison with the corresponding ARPES [1] as well as XAS and XMCD [2,3] experimental data.

[1] J. Sanchez-Barriga et al., Nat. Communications, submitted (2015) [2] A. Ney et al., in preparation [3] J. Honolka et al., in preparation

Talk O 62.12 Wed 18:15 H24

Trions in a carbon nanotube from ab-initio many-body perturbation theory — •Thorsten Deilmann, Matthias Drüppel, and Michael Rohlfing — Institut für Festkörpertheorie, Universität Münster, Germany

Trion states of three correlated particles (e.g. two electrons and one hole) show up in the optical spectra of doped or gated nanostructures, like carbon nanotubes or transition-metal dichalcogenides.
We demonstrate that trions can be described within ab-initio many-body perturbation theory, as a natural extension of the widely used *GW* method and Bethe-Salpeter equation. This allows for a direct comparison with excitons on equal footing.
We investigate trion states in a semiconducting $(8, 0)$ carbon nanotube, and discuss their spectra, composition, and wave functions. Luminescence from the trions is red-shifted by $\sim 135\,\mathrm{meV}$ compared to the excitons.

O 66: Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Wednesday 18:15–20:30 Poster A

Poster O 66.1 Wed 18:15 Poster A

Improving anharmonic vibrational calculations from first principles — •Joseph C.A. Prentice, Bartomeu Monserrat, and Richard J. Needs — TCM Group, Cavendish Laboratory, University of Cambridge, UK

The vibrational self-consistent field (VSCF) method, as described in PRB 87 144302, has had several successes in accurately calculating the anharmonic properties of various materials, such as diamond, ice and solid hydrogen. However, a practical issue with the method is the large number of DFT calculations required to map the Born-Oppenheimer energy surface sufficiently accurately. We look at improvements to the method that reduce this computational load, in particular using data on forces from DFT calculations to improve the accuracy of the mapping. Results using this improved method are presented for competing structures of silicate perovskite under lower mantle conditions. Further improvements, involving the inclusion of n-body coupling between phonons, and their possible implementation are also discussed.

Poster O 66.2 Wed 18:15 Poster A

Towards a practical implementation of second-order Møller-Plesset perturbation theory for solids — •Xiangyue Liu, Arvid Conrad Ihrig, Sergey Levchenko, Igor Ying Zhang, and

Matthias Scheffler — *Fritz-Haber-Institut der MPG, Berlin, DE*

The second-order Møller-Plesset perturbation theory (MP2) method is gaining attention in materials science, because it is free from the one-electron self-interaction error. Such error, as a lasting problem in density-functional theory, can lead to a wrong prediction of electronic band gaps, charge transfers, and reaction barriers, all of which are ubiquitous electronic properties or behaviors in condensed-matter systems. However, the unfavourable computational complexity, especially the cubic scaling with respect to the $\boldsymbol{k}$-point number in reciprocal space, limits the applicability of MP2 for solids. In this project we present a practical MP2 implementation for solids in the all-electron full-potential framework. In our implementation, the MP2 correlation energy is evaluated in the atomic-orbital (AO) representation (AO-MP2), which allows for a lower computational scaling in both real and reciprocal spaces[1]. The localized resolution of identity (RI-LVL) technique[2] is adopted to address the memory bottleneck of the AO-MP2 method, making it feasible to handle systems with several hundred atoms per supercell while avoiding the reliance on the disk storage. We demonstrate the accuracy as well as the efficiency of our new MP2 implementation for a diverse set of materials. [1] Levchenko, S. V. *et al.*, Comput. Phys. Comm. **192**, 60, (2015); [2] Ihrig, A.C. *et al.*, New J. Phys. **17** 093020, (2015).

Poster O 66.3 Wed 18:15 Poster A

Application of the exact exchange functional to magnetic metals within the FLAPW method — •Max Nusspickel[1], Markus Betzinger[1], Christoph Friedrich[1], Andreas Görling[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

Orbital-dependent functionals form a promising class of exchange-correlation (xc) functionals in Kohn-Sham density-functional theory. Already the simplest functional of its kind, the exact exchange functional (EXX), cures the unphysical Coulomb self-interaction error of LDA and GGA functionals. In order to obtain a local xc potential from an orbital-dependent functional, the optimized effective potential (OEP) method is used, resulting in an integral equation for the potential. This equation, however, determines the potential only up to a constant.

In spin-polarized metals, the alignment of the spin-up and spin-down potentials is obtained by the requirement of electron number conservation: variations of the potential can lead to a change of the Fermi energy and, hence, to a variation of the densities of both electron spins. In this way, the OEP equations for the spin-up and spin-down potentials are coupled and the spin-dependent xc potential is obtained from a single OEP equation. We discuss the extension of our EXX-OEP implementation within the linearized augmented plane-wave (FLAPW) method and show results for prototype magnetic metals.

Poster O 66.4 Wed 18:15 Poster A

Electric switchable giant Rashba-type spin splitting in bulk PbS — •Bin Shao[1], Wenhui Duan[2], and Thomas Frauenheim[1] — [1]BCCMS, University of Bremen, Bremen, Germany — [2]Institute for Advanced Study, Tsinghua University, Beijing, China

Realizing electric controllable spin is one of the major challenges in the field of spintronics. A promising approach is to utilize so-called Rashba effect, which arises from the spin-orbit coupling under broken inversion symmetry, leading to a momentum-dependent spin splitting in k-space. However, the sizes of this splitting are usually rather small, which hinders the application of this effect in spintronics. In this work, based on density functional calculation, we predict a giant Rashba-type spin splitting in bulk PbS with space group $P6_3mc$. The phonon spectrum calculation gives evidence of the thermal stability of this system. The origin of the giant Rashba effect has been demonstrated from the deviation of the S ion from the inversion symmetric position, leading to an ferroelectric polarization along c axis. By switching the direction of the ferroelectric polarization, the spin directions of bulk carriers governed by the Rashba effect are completely rotated, which grants a potential approach to manipulate the spin of electrons by an external electric field. Moreover, under a reasonable hydrostatic pressure, the system could obtain the inversion symmetry due to the movement of the S ion backwards to symmetric positions. As a result, the system turns into a topological phase with the massless Dirac cone state at the (001) surface.

Poster O 66.5 Wed 18:15 Poster A

GW+fRG: Towards an fRG enhancement of ab initio calculations — •Jannis Ehrlich[1,2], Carsten Honerkamp[1], Christoph Friedrich[2], and Stefan Blügel[2] — [1]Institut für theoretische Festkörperphysik, RWTH Aachen University, D-52056 Aachen, Germany — [2]PGI-1 and IAS-1, FZJ & JARA, D-52425 Jülich, Germany

Spin excitations in solids are of fundamental interest for a wide variety of phenomena. Most materials-specific theoretical studies are based on the adiabatic treatment of the spin-degees of freedom in the context of DFT. Approaches based on the *GW* approximation include screening effects due to charge fluctuations but neglect vertex corrections and other contributions like magnetic fluctuations. The functional renormalization group (fRG) can overcome these limitations as it resums a different class of diagrams, among them charge and magnetic fluctuations and vertex corrections. We discuss how the equations for two-particle vertices in the fRG contain the *GW* approximation, the Bethe-Salpeter equation (BSE) and the parquet approach on certain levels of approximations. Thus, a fRG calculation of materials properties could be a powerful approach to improve the *GW* and BSE methods already applied in first-principles calculations. By using recently suggested channel decomposition schemes [1,2] the method has gained in flexibility and in potential for tackling more complex tasks. Here we propose first steps to develop the fRG approach for the *ab initio* calculation of materials properties.

[1] C. Husemann, M. Salmhofer, Phys. Rev. B **79**, 195125 (2009).
[2] W. Wang *et al.*, Phys. Rev. B **85**, 035414 (2012).

Poster O 66.6 Wed 18:15 Poster A

The quantum anomalous Hall effect in HgMnTe — •Jan Böttcher, Christoph Kleiner, and Ewelina M. Hankiewicz — Uni Würzburg, Institut für Theoretische Physik und Astrophysik, Germany

Recently, the quantum anomalous Hall (QAH) effect was predicted to exist in Mn doped HgTe. Within the QAH phase only one edge state remains at an edge due to an opposite coupling of spin to the magnetization. The experimental proof is however still outstanding. The paramagnetic nature of the Mn impurities gives rise to the formation of Landau levels which makes it experimentally challenging to distinguish the QAH from a conventional quantum Hall (QH) state. Based on the BHZ model, we present an extended study of the transition from the quantum spin Hall to the QAH state as well as the QAH to the quantum Hall state. For this purpose, we make use of the finite difference method and compare the results with analytical calculations. Hallmarks of the QAH states in the presence of magnetic fields are discussed. The BHZ model has natural limitations in the high magnetic field regime. We therefore compare our results with band structure calculations based on the 8x8 Kane Hamiltonian. Signatures in the magnetoresistance are discussed which might open the door to distinguish the QAH from the QH state in future transport experiments.

We acknowledge financial support by the DFG within SFB 1170 "ToCoTronics".

Poster O 66.7 Wed 18:15 Poster A

Nonconventional screening of the Coulomb interaction in low-dimensional semiconductors and insulators — Ersoy Sasioglu, •Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Screening effects play a fundamental role in determining the exciton binding energy, electron dynamics, and the effective electron-electron interaction in low-dimensional semiconductors and insulators. Experimental observation of the large exciton binding energies and nonhydrogenic Rydberg series in low-dimensional semiconductors indicate an unusual non-local screening of the Coulomb interaction. By means of first-principles calculations in conjunction with the random-phase approximation (RPA) within the FLAPW method we study the screening of the Coulomb interaction in low-dimensional semiconductors and insulators. For this purpose a novel tetrahedron method has been implemented. We show that the screening in these systems deviates substantially from the bulk behavior, i.e., the screened interaction W cannot be expressed by a simple static dielectric constant. We compare the numerical RPA results to analytical functions derived from image-charge models for the isolated slab and for a repeated slab model. We find a nonconventional screening in low-dimensions. This nonconventional screening explains the deviations from the usual hydrogenic Rydberg series of energy levels of the excitonic states in one- and two-dimensional semiconductors and opens up possibilities for fundamental studies of correlation effects in low-dimensional materials.

O 80: Frontiers of Electronic Structure Theory: Focus on Topology and Transport IV

Thursday 10:30–13:15 H24

Topical Talk O 80.1 Thu 10:30 H24

Transport phenomena in broken-symmetry metals: Geometry, topology, and beyond — •Ivo Souza — Universidad del País Vasco, San Sebastián, Spain

While topological quantization is usually associated with gapped systems – Chern insulators and topological insulators – it can also occur in broken-symmetry metals, where the Fermi surface (FS) consists of disjoint sheets: the Berry-curvature flux through each sheet is quantized, defining an integer Chern index. Using ferromagnetic bcc Fe as an example, I will describe how the FS Chern numbers are related to the chiral degeneracies ("Weyl points") in the bandstructure. When placed in a static magnetic field, a Weyl (semi)metal will display the chiral magnetic effect (CME), where an electric field pulse $\mathbf{E} \parallel \mathbf{B}$ drives a transient current $\mathbf{j} \parallel \mathbf{B}$. Weyl semimetals with broken inversion and mirror symmetries can also display a "gyrotropic magnetic effect" (GME), where an oscillating magnetic field drives a current and, conversely, an electric field induces a magnetization. The GME is the low-frequency limit of natural optical activity. It is governed by the intrinsic magnetic moment (orbital plus spin) of the Bloch electron on the FS, in much the same way that the anomalous Hall effect and CME are governed by the FS Berry curvature. Like the Berry curvature, the intrinsic magnetic moment should be regarded as a basic ingredient in the Fermi-liquid description of transport in broken symmetry metals.

Topical Talk O 80.2 Thu 11:00 H24

Dirac Fermions in Antiferromagnetic Semimetal — •Peizhe Tang, Quan Zhou, Gang Xu, and Shou-Cheng Zhang — Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA

The analogues of elementary particles in condensed matter systems have been extensively searched for because of both scientific interests and technological applications. Recently massless Dirac fermions are found to emerge as low energy excitations in the materials named Dirac semimetals. The currently known Dirac semimetals are all nonmagnetic with both time-reversal symmetry T and inversion symmetry P. Here we show that Dirac fermions can exist in one type of antiferromagnetic systems, where T and P are broken but their combination PT is respected. We propose orthorhombic antiferromagnet CuMnAs as a candidate, analyze the robustness of the Dirac points with symmetry protections, and demonstrate its distinctive bulk dispersions as well as the corresponding surface states by ab initio calculations. Our results give a new routine towards the realization of Dirac materials, and provide a possible platform to study the interplay of Dirac-related physics and magnetism.

Talk O 80.3 Thu 11:30 H24

Spin Hall effect in non-collinear antiferromagnets Mn3X (X=Sn, Ge, Ga) — •Yang Zhang[1,3], Yan Sun[1], Claudia Felser[1], and Binghai Yan[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — [2]Max Planck Institute for the Physics of Complex Systems, 01187 Dresden, Germany — [3]Leibniz Institute for Solid State and Materials Research, 01069 Dresden, Germany

Recently, large anomalous Hall effect (AHE) was realized in noncollinear antiferromagnetic (AFM) compounds Mn3X (X=Sn, Ge, Ga). We have found that the nonzero Berry curvature – origin of the AHE observed – will lead to another topological effect, the spin Hall effect (SHE) in the titled compounds. We have systematically investigated the intrinsic SHE and revealed large spin Hall conductivity [~1000 ((*/e)*(S/cm)], which is comparable to that of the well-know SHE material Pt. Our work present a new family of AFM compounds for the room-temperature spintronic applications.

Talk O 80.4 Thu 11:45 H24

Electronic reconstruction and anomalous Hall conductivity in 3*d*-oxide honeycomb lattices within the corundum structure — •santu baidya and rossitza pentcheva — Fakultät für Physik and Center of Nanointegration (CENIDE), Universität Duisburg-Essen, 47057 Duisburg

The electronic structure of 3*d* transition metal oxide honeycomb layers confined in the corundum structure (α-Al_2O_3) along the [0001] direction is investigated using density functional theory including an on-site Coulomb term (GGA+U). While in some cases (e.g. $(M_2O_3)/(Al_2O_3)_5$, M=Fe, Co, V, Cr, Ni) the confined geometry preserves the magnetic and electronic ground state properties of the corresponding bulk corundum compound M_2O_3, strong deviations from the bulk behavior are observed in the case of Ti_2O_3 and Mn_2O_3 bilayers. Our results indicate a formation of a quasi two-dimensional electron gas with a vertical confinement of ∼5 Å for Ti_2O_3 and ∼8.5 Å for Mn_2O_3. As a function of lateral strain $(Ti_2O_3)/(Al_2O_3)_5$ undergoes a metal-to-insulator transition associated with a switching of orbital polarization. In the metallic state the Dirac point can be tuned to the Fermi level by variation of the c/a ratio. Including spin-orbit coupling a finite anomalous Hall conductivity is observed in $(M_2O_3)/(Al_2O_3)_5$ (M=Ti, Mn).

Talk O 80.5 Thu 12:00 H24

Anomalous hall effect in triangular antiferromagnetic ordered structure — •Hao Yang[1], Sun Yan[2], Felser Claudia[2], Parkin Stuart[1], and Binghai Yan[2] — [1]Max Planck Institute of Microstructure Physics, 06120 Halle(Saale), Germany — [2]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The anomalous Hall effect (AHE), a fundamental transport phenomenon of electrons in solids, has been believed to appear in ferromagnetic materials. Very recently AHE is revealed in noncollinear antiferromagnetic compounds. In this work, we have systematically investigated the AHE in antiferromagnetic materials Mn3X (X=Ir, Ge, Sn, Ga), where noncollinear 120-degree type antiferromagnetic spin order exists in the quasi-layered lattice. Assisted by the symmetry analysis, we demonstrate the strong anisotropy of the intrinsic anomalous Hall conductivity that is determined by the Berry curvature in the band structure. Our work well interprets recent experiment observations and predicts novel antiferromagnetic material candidates for the spintronic application.

Talk O 80.6 Thu 12:15 H24

Anomalous Hall conductivity and orbital magnetization as local quantities — •Antimo Marrazzo[1] and Raffaele Resta[2] — [1]THEOS, EPF Lausanne, Switzerland — [2]Dipartimento di Fisica, Univ. Trieste, Italy

Anomalous Hall conductivity (AHC) and orbital magnetization (OM) are—from a theorist's viewpoint—closely related: both have an expression as **k**-space integrals of the appropriate geometrical quantity. The **k** space is an artificial construct: all bulk properties are embedded in the ground state density matrix in **r** space, independently of the boundary conditions. Is it possible to address AHC and OM as local properties, directly in **r** space? For insulators, two recent papers have proved that the answer is affirmative: both AHC (quantized in insulators) and OM can be evaluated from a local formula over bounded samples. A rationale can be found in the "nearsightedness" of the density matrix: but since this is *qualitatively* different in insulators and metals (exponential vs. power law) it is not obvious that the same successful approach can be extended to metals. Using model Hamiltonians, we have performed simulations over 2D bounded metallic flakes, where the T-invariance is broken in two alternative ways: either à la Haldane, or by a macroscopic **B** field. In both cases, our simulations show that the relevant quantity can be extracted from a knowledge of the electron distribution in the bulk region of the sample only. This looks counterintuitive because the OM of a magnetized sample owes to currents localized near its surface; but the key reason for the success of the local approach to AHC and OM is that the formulas are *not* based on currents.

Talk O 80.7 Thu 12:30 H24

Laser induced DC photocurrents in a Topological Insulator thin film — •Thomas Schumann[1], Nina Meyer[1], Gregor Mussler[4], Eva Schmoranzerová[2], Dagmar Butkovicova[2], Helena Reichlová[3], Lukas Braun[5], Christian Franz[6], Michael Czerner[6], Pertr Němec[2], Detlev Grützmacher[4], Tobias Kampfrath[5], Christian Heiliger[6], and Markus Münzenberg[1] — [1]IfP, EMA University Greifswald, Germany — [2]MFF, Charles University, Prague, Czech Republic — [3]FZU, Prague, Czech Republic — [4]PGI-9, Jülich, Germany — [5]FHI Berlin, Germany — [6]University of Gießen, Germany

Topological Insulators (TI) open up a new route to influence the transport of charge and spin in a surface film via spin-momentum locking [1,2]. It has been demonstrated experimentally [2] that illumination by circularly polarized light can result in excitation of a helicity-dependent

photocurrent.We report our recent results on laser induced photocurrents in a terniary 3D TI thin film. The resulting photocurrents are classified after [1,2] and we show that there are at least two signals visible, for example in time dynamics, which behave different in the suggested parameters.

We acknowledge the funding of the DFG via the SPP 1666 Topological Insulators and the joint DAAD PPP Czech Republic project FemtomagTopo. [1]S.D.Ganichev,W.Prettl,J.Phys.: Condens. Matter 15 (2003) R935-R983

[2]J.W.McIver,D.Hsieh,H.Steinberg,P.Jarillo-Herrero and N.Gedik, Nature Nanotechnology 7, 96-100 (2012)

Talk O 80.8 Thu 12:45 H24

Robustness of exchange protocols of Majorana fermions in quantum wire networks — •Christian Tutschku[1], Rolf W. Reinthaler[1], Chao Lei[2], Allan H. MacDonald[2], and Ewelina M. Hankiewicz[1] — [1]Faculty of Physics and Astrophysics, University of Würzburg, Würzburg, Germany — [2]Department of Physics, University of Texas at Austin, USA

The interface between topological non-trivial, one-dimensional, spinless p-wave superconductors and the vacuum is connected to the appearance of Majorana edge-modes [1], whose non-trivial exchange statistics makes them promising candidates for topological quantum computation [2]. Via T-Bar structures build of 1D-nanowires we can manipulate and exchange the Majorana fermions by purely electrical means [3]. By applying a tight binding approach we solve the time dependent Bogoliubov-de Gennes equations for the Kitaev chain model [1] and also cure the problem of an appearing additional Majorana-boundstate located at the T-Bar crossing point for small lattice constants. Furthermore we analyze how the robustness of the exchange protocols is affected by non-adiabatic effects or by a finite overlap of the Majorana bound states.

We acknowledge financial support by the DFG within SFB 1170 ToCoTronics.

[1] A. Y. Kitaev, Physics-Uspekhi **44**, 131 (2001)
[2] D. A. Ivanov, PRL **86**, 268 (2001)
[3] J. Alicea et al., Nature Physics **7**, 412 (2011)

O 88: Frontiers of Electronic Structure Theory: Focus on Topology and Transport V

Thursday 15:00–18:15 H24

Talk O 88.2 Thu 15:15 H24

All-Electron Many-Body Approach to X-Ray Absorption Spectroscopy — •Christian Vorwerk, Caterina Cocchi, and Claudia Draxl — Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin, Germany

We present an all-electron approach of the many-body perturbation theory to describe X-ray absorption spectroscopy (XAS) in solid-state materials. In this formalism, the electron-hole interaction is explicitely included by solving the Bethe-Salpeter equation. A fully relativistic description of core states, as implemented in the all-electron full-potential code `exciting`[1], enables the explicit treatment of the effects of spin-orbit coupling in the spectra. We investigate the XAS for prototypical systems, such as TiO_2 and MgO, considering excitations from oxygen K and metal L edges. Our results, in good agreement with experiments, allow us to gain insight into the nature of the core-level excitations of these materials.

[1] A. Gulans et al., J. Phys. Condens. Matter 26, 363202 (2014).

Talk O 88.3 Thu 15:30 H24

Cohesive properties from all-electron RPA total energies — •Markus Betzinger[1], Christoph Friedrich[1], Andreas Görling[2], and Stefan Blügel[1] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Germany

We present an all-electron implementation of the RPA total energy within the full-potential linearized augmented plane-wave (FLAPW) method. An incomplete basis-set correction (IBC) [1] is employed to improve the convergence of the total energy with respect to the basis-set and the number of unoccupied states. To some extent the IBC incorporates an infinite number of bands and enables a virtually exact treatment of the core electrons.
We demonstrate that the core electrons give rise to a sizeable contribution to the RPA total energy. Their individual contribution is comparable to that of the valence electrons. All-electron RPA lattice constants and bulk moduli are shown for a set of prototype materials and compared to experimental results. An excellent agreement with experiment is observed.
[1] M. Betzinger *et al.*, Phys. Rev. B (accepted, 2015); **88**, 075130 (2013); **85**, 245124 (2012).

Talk O 88.4 Thu 15:45 H24

Explicitly correlated self consistent field theory — •Christian Lasar and Thorsten Klüner — Universität Oldenburg

Explicitly correlated correlation methods are an interesting field of current research since they are able to drastically improve the otherwise slow basis set convergence of conventional correlation methods. Therefore, chemical accuracy can be achieved with rather small basis sets.[1] The new correlation method presented in this contribution has already been developed for two-electron systems a long time ago[2]. We present the generalization of this ansatz to N-electron systems.

The basic idea is to augment a single slater-determinant with an explicitly correlated prefactor which then takes care of the correlation effects and the basis set convergence. Another interpretation of this ansatz would be a contracted CISD with orbital optimization in a complete basis set. The contraction is achieved by the explicitly correlated prefactor whose choice therefore defines the possible accuracy of the method. In principle, the generalization to any pair method i.e. CCSD and MP2 will be possible.

The big advantage of this kind of ansatz for the wave function is the drastic reduction of matrix elements needed for the optimization of the wave function. As a result, the presented method will be applicable to large molecules.

[1] Chem. Rev. 112, p. 4 (2012) [2] J. Chem. Phys. 99, p. 8830 (1993)

Talk O 88.5 Thu 16:00 H24

Representing energy landscapes by combining neural networks and the empirical valence bond method — •Sinja Klees[1], Ramona Ufer[2], Volodymyr Sergiievskyi[2], Eckhard Spohr[2], and Jörg Behler[1] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Theoretische Chemie, Universität Duisburg-Essen, D-45141 Essen, Germany

In recent years, artificial neural networks (NNs) have become a powerful method to develop reactive interatomic potentials for large systems. However, the construction of NN potentials can become computationally very demanding due to the high dimensionality of the configuration space, which needs to be mapped by reference electronic structure calculations. Combining NN potentials with the empirical valence bond (EVB) method offers a promising approach to derive the potential energy of complex systems with substantially reduced effort, since the size of the reference structures can be strongly decreased. Preliminary results will be discussed and compared to density functional theory data.

Talk O 88.6 Thu 16:15 H24

CELL: a python package for cluster expansions with large parent cells — •Santiago Rigamonti[1], Maria Troppenz[1], Christopher Sutton[2], Luca M. Ghiringhelli[2], and Claudia Draxl[1] — [1]Humboldt-Universität zu Berlin — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft

The discovery of new materials for applications in areas such as energy harvesting, relies more and more on the accurate theoretical description of complex structures with large unit cells. The properties of interest are often tuned by substitutional dopants. Due to the vast configurational dopant space, a wide-spread approach is the cluster expansion (CE) technique. Most available CE codes are designed for alloys based on small parent cells, with usually 1 to 4 atoms. For the many important materials with much larger parent cells such approaches can't be applied. We devise an iterative scheme, based on efficient samplings of the configurational space, avoiding full structure enumerations. CELL consists of several modules that can be used independently, enabling to design CEs for specific purposes. Various CE schemes are available, offering ℓ_2 and ℓ_1 norms as penalization terms and different

cross-validation strategies. Methods such as LASSO and split Bregman iteration are available for dealing with the ℓ_1 norm (compressive sensing). Access to finite-temperature properties and the characterization of phase transitions is possible through the Wang-Landau and diffusive nested sampling modules. Examples are presented for type-I thermoelectric clathrates, with 46 sites in the parent cell.

Talk O 88.7 Thu 16:30 H24

Structural and electronic properties of the thermoelectric clathrates $Ba_8Al_xSi_{46-x}$ and $Sr_8Al_xSi_{46-x}$ — •Maria Troppenz, Santiago Rigamonti, and Claudia Draxl — Humboldt-Universität zu Berlin

Clathrate compounds are promising candidates for high-efficiency thermoelectric applications. Their cage-like structure containing guest atoms allows for exploiting the idea of the phonon-glass electron-crystal and reaching a large figure of merit. We study $Ba_8Al_xSi_{46-x}$ and $Sr_8Al_xSi_{46-x}$ ($6 \leq x \leq 16$), where optimal electronic properties are expected close to the Zintl composition ($x = 16$). Cluster expansions on various quantities are performed, thus having access to ground-state as well as finite-temperature properties. A linear increase of the lattice constant with the number of Al substituents is obtained (0.019 Å per Al addition) confirming experimental observations (0.02 Å). The calculated bond distances between high-symmetry sites agree well with experiment for the full compositional range [1,2]. We find a close correlation between bond distances and fractional Al occupancies. This helps improving models used by experimentalists to estimate fractional occupancies. The substitutional configurations present an order-disorder transition around $600 - 900$ K, which is further analyzed applying the Wang-Landau method. An important finding is the semiconducting behavior of the low-temperature ordered phase at the Zintl composition, which points out the technological relevance of these compounds.

[1] J. H. Roudebush *et al.*; *Inorg. Chem.* **51**, 4161 (2012)
[2] M. Bobnar *et al.*; *Dalton Trans.* **44**, 12680 (2015)

Talk O 88.8 Thu 16:45 H24

***Ab-initio* calculation of Raman spectra of graphene-based materials** — •Albin Hertrich, Caterina Cocchi, Pasquale Pavone, and Claudia Draxl — Department of Physics, Humboldt-Universität zu Berlin, Germany

Raman scattering is an important non-destructive method for characterizing carbon-based materials. The main features of experimental Raman spectra of pristine graphene and graphite are the first-order G-band at ≈1580 cm^{-1} and the dispersive second-order 2D-band at ≈2700 cm^{-1}. We calculate first- and second-order Raman spectra fully *ab-initio* using the full-potential all-electron DFT package `exciting` [1], which allows for the calculation of both phonon dispersion, within the frozen-phonon approximation, and frequency-dependent dielectric tensors, from time-dependent DFT and the Bethe-Salpeter equation. In our approach [2], we expand the dielectric tensor with respect to the phonon normal coordinates. By taking its derivatives and by computing vibrational matrix elements, we calculate Raman scattering intensities. Applying this scheme to monolayer graphene, bilayer graphene, and graphite, we obtain the G-band in good agreement with experiment [3]. Furthermore, we explore the influence of both the stacking sequence and the laser energy on the 2D-band.

[1] A. Gulans *et al.*, J. Phys.: Condens. Matter **26**, 363202 (2014).
[2] C. Ambrosch-Draxl *et al.*, Phys. Rev. B **65**, 064501 (2002).
[3] A. C. Ferrari *et al.*, Phys. Rev. Lett. **97**, 187401 (2006).

Talk O 88.9 Thu 17:00 H24

Exciton dispersion in layered and 2D systems — •Francesco Sottile[1,2], Giorgia Fugallo[1,2], Pierluigi Cudazzo[1,2], and Matteo Gatti[1,2,3] — [1]Laboratoire des Solides Irradiés, École Polytechnique, CNRS, CEA-IRAMIS, Université Paris-Saclay, F-91128 Palaiseau, France — [2]European Theoretical Spectroscopy Facility — [3]Synchrotron SOLEIL, L'Orme des Merisiers, Saint-Aubin, Boîte Postale 48, F-91192 Gif-sur-Yvette, France

The study of the exciton dispersion is of paramount importance for all applications involving light harvesting, beside providing fundamental knowledge about exciton mobility and migration. Using state-of-the-art ab initio many-body approach, like the Bethe-Salpeter equation [1], we present a first principle study of exciton dispersions in layered materials and 2D systems. Results for the former systems (on the prototypical hBN and MoS2) have been recently confirmed by experiments carried out at the Synchrotron ESRF [2]. For the latter (2D) systems we investigate exciton dispersion in graphane and hBN. From our results we provide a general picture of the mechanisms governing the dispersion of neutral excitations in 2D systems, and of the role played by the confinement of the electronic charge in setting the exciton binding energy. In particular we found that due to the strongly reduced screening of the Coulomb interaction in low- dimensional materials, the binding energy of both Wannier and Frenkel excitons in the optical spectra is large and comparable in size[3]. [1] M. Gatti et al., Phys. Rev. B 88, 155113 (2013) [2] G. Fugallo et al. Phys. Rev. B 92, 165122 (2015) [3] P. Cudazzo et al. submitted to Phys. Rev. Lett.

Talk O 88.10 Thu 17:15 H24

Electronic structure of selected superheavy elements (Z¿104) — •Hana Cencarikova[1] and Dominik Legut[2] — [1]Institute of Experimental Physics, SAS, Kosice, Slovakia — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

The electronic structure of selected super-heavy elements (Z¿104) have been determined from the first-principle calculations based on the density functional method. To determine the ground-state structure we have calculated number of basic phases including the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures. Our results were obtained using local density approximation for the exchange and correlation effects and without and with the spin-orbit interaction for the band states. The analysis has been focused on the determination of the electronic density of states, electronic band structure dispersion relation, mechanical properties (elastic constants) and selected thermodynamical properties.

Talk O 88.11 Thu 17:30 H24

Layer-resolved calculated vibrations at gold surfaces — •Andrei Postnikov[1] and Kamil Moldosanov[2] — [1]Université de Lorraine, LCP-A2MC, Metz, France — [2]Kyrgyz-Russian Slavic University, Bishkek, Kyrgyzstan

Vibration modes at (001), (011) and (111) surface of gold are calculated from first principles, using the Siesta method [1] and the frozen phonon approach. Calculations are done on thick slabs of moderate lateral size – (2×2) for (001), (2×3) for (011), (3×3) for (111). This allows to resolve the vibration patterns layer by layer into the depth, in dependence on the in-plane wavevector component, and discriminating the polarisation of vibration modes. One notes the softening of modes at the surface, and an appearance of specifically surfacial modes. The bulk behaviour is largely recovered from the 5th or 6th layer downwards.

This study was driven by an intention to grasp the properties of longitudinal acoustic modes propagating at some depth under the surface of gold nanoparticles, which were an important element of our recent work related to the mechanism of radiofrequency absorption and hence resulting heating of nanoparticles of $\gtrsim 5$ nm size [2]. Since it is difficult to meaningfully incorporate the diversity of the nanoparticles' shapes in a practical calculation, the vibrations beneath the most common facets occurring at the nanoparticles' surface were studied instead.

1. The Siesta method, `http://departments.icmab.es/leem/siesta/` .
2. A. Postnikov and K. Moldosanov, `http://arxiv.org/abs/1508.00735` .

Talk O 88.12 Thu 17:45 H24

Electronic structure, mechanical and thermodynamic properties of Actinium from first-principles — •Barbora Kacerovska[1] and Dominik Legut[2] — [1]Nanotechnology, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic — [2]IT4Innovations Center, VSB-TU Ostrava, CZ 708 33 Ostrava, Czech Republic

In this work, the mechanical (elastic constants) and thermodynamic properties of actinium were investigated using first-principle calculations. Our results were obtained using density functional theory employing local density and general gradient approximation for the electronic exchange-correlation effects and including the spin-orbit interaction for the band states. The ground-state structure were determined among simple phases like the face-centered cubic, body-centered cubic, simple cubic as well as hexagonal closed packed structures.

Talk O 88.13 Thu 18:00 H24

Interaction of Tritium and Chlorine 36 with defects in Graphite: Insights from Theory — •Christoph Lechner[1], Philippe Baranek[1], and Holger Vach[2] — [1]EDF Lab Les Renardières, Avenue des Renardieres, F-77818 Moret-sur-Loing Cedex, France — [2]CNRS-LPICM, Ecole Polytechnique, F-91128 Palaiseau Cedex, France

In order to optimize the waste management of nuclear graphite used in power plants, it is important to understand the properties of the activated impurities it contains, such as tritium and chlorine 36. There-

fore, a computational study of the interaction of tritium and chlorine 36 with defects in graphite has been achieved at the density functional theory (DFT) level by using the functionals PBE and PBE0 with Grimme's D3 dispersion correction. The physisorption and chemisorption of atomic and molecular hydrogen or chlorine on graphite surfaces, (001), (100), and (110) with or without mono- and divacancies, have been investigated. The stabilities of the formed complexes are interpreted in terms of the formation energy. To obtain insight into the nature of the bonding a population analysis of the systems has been performed. While the bonding of hydrogen is mostly covalent for chemisorption and van der Waals for physisorption, the behavior of chlorine is much more complex. Depending on the defect site, both, dominantly covalent and dominantly charge transfer bonding, is observed. Raman spectra for selected structures have been investigated, in order to evaluate, if the experimentally observed defect bands can be reproduced.

O 99: Symposium on Frontiers of Electronic Structure Theory: Focus on Topology and Transport

Friday 09:30–12:15 H1

Invited Talk O 99.1 Fri 9:30 H1

Intrinsic Transport Coefficients and Momentum Space Berry Curvatures — •Allan H MacDonald — University of Texas at Austin, Austin TX, USA

The response of a conductor to a bias voltage is normally dominated by repopulation of states near the Fermi level. The transport steady state is fixed by a competition between acceleration in an electric field and disorder-induced scattering which attempts to restore equilibrium. This response of observables to a bias voltage is therefore extrinsic. There is however also response of states away from the Fermi level, which are polarized by the electric field. Provided that the typical band separation is larger than the finite life-time uncertainty in Bloch state energies this response is intrinsic, and for some observables it can be dominant. Intrinsic response coefficients are attractive targets for electronic structure theory because they are readily evaluated. Examples of responses to bias voltages that are sometimes dominantly intrinsic are the anomalous Hall conductivity of ferromagnetic or antiferromagnetic conductors, the spin-Hall conductivity of heavy metals, and current-induced torques in heavy-metal/ferromagnet systems. Intrinsic transport coefficients tend to be large in crystals with large momentum-space Berry curvatures, for example in crystals with topologically non-trivial electronic structure, and remain finite when a gap opens at the Fermi level to eliminate the Fermi surface. I will discuss some important examples of transport coefficients that are dominated by intrinsic contributions, mentioning as an important case the quantum anomalous Hall effect.

Invited Talk O 99.2 Fri 10:00 H1

Berry phase linked spin-orbit torques in Ferromagnetic and Antiferromagnetic systems — •Jairo Sinova — Johannes Gutenberg Universität Mainz, Staudingerweg 7, 55128 Mainz Germany

As current-driven torques are becoming more relevant in future MRAM technologies, in-plane current magnetization dynamics driven by the so called Rashba spin-orbit torques or through a combination of spin-Hall effect and spin-transfer torque has become more and more important. Understanding these torques is paramount to maximize their use. In recent experiments we have shown that in addition to the intrinsic SHE and STT effect there exists an intrinsic spin-orbit torque originating from the Berry phase of the spin-orbit coupled Bloch electrons analogous to the intrinsic spin Hall effect. This type of torques can be observed through SO-FMR driven experiments. We show this new type of toques in theory and experiments in GaMnAs and show that it can be of similar strength to the strong field-like torque. In addition, we extend these physics to a new type of order-parameter manipulation by currents by examining the combined effect of spin-orbit coupling and anti-ferromagnetic order. We show that in broken inversion symmetry anti-ferromagnets a current will induced a non-equilibrium Néel-order field that will act directly on the Néel order parameter, hence making the direct manipulation of anti-ferromagnets without auxiliary exchange biased coupling to other ferromagnets a new and exciting possibility. One of these type of Néel torques has been recently experimentally confirmed.

Invited Talk O 99.3 Fri 10:30 H1

Transport in Topological Insulators and Topological Superconductors: In Search of Majorana Fermions — •Ewelina Hankiewicz — Wuerzburg University

Topological insulators (TIs) have a bulk energy gap that separates the highest occupied band from the lowest unoccupied band and the metallic gapless states at the edge [1]. Similarly, topological superconductors (TSC) have gapless zero energy states protected by the particle-hole symmetry, which in some cases form Majorana bound states. Here, we focus on the proximity-induced superconductivity in TIs [2] as well as on unusual properties of TSC [3] showing that they both can pave a road to find a Majorana state.

Concerning proximity-induced superconductivity in TIs, we describe a novel superconducting quantum spin-Hall effect, which is protected against elastic backscattering by combined time-reversal and particle-hole symmetry even in magnetic fields [2]. We discuss unusual transport properties of this effect and possible Majorana detection schemes.

Finally, we discuss new systems like TSC on the hexagonal lattices. We develop combined microscopic and macroscopic description of these materials that predicts realistic scanning tunneling microscopy signal in these superconductors [3]. Is there a way to measure Majorana state in these systems?

[1] G. Tkachov and E. M. Hankiewicz, Review in Phys. Status Solidi B 250, 215 (2013). [2] R. Reinthaler, G. Tkachov and E.M. Hankiewicz, Phys. Rev. B 92, 161303(R) (2015). [3] L. Elster, C. Platt, R. Thomale, W. Hanke, and E. M. Hankiewicz, Nature Comm. 6, 8232 (2015).

session break

Invited Talk O 99.4 Fri 11:15 H1

Engineering Topological Quantum States: From 1D to 2D. — •Jelena Klinovaja — University of Basel, Switzerland

I will discuss low-dimensional condensed matter systems, in which topological properties could be engineered per demand. Majorana fermions can emerge in hybrid systems with proximity pairing in which the usually weak Rashba spin-orbit interaction is replaced by magnetic textures. I will discuss candidate materials such as semiconducting nanowires [1] and atomic magnetic chains [2]. One further goal is to go beyond Majorana fermions and to identify systems that can host quasiparticles with more powerful non-Abelian statistics such as parafermions in double wires coupled by crossed Andreev reflections [3,4]. Next, I will focus on 'strip of stripes model' consisting of weakly coupled one-dimensional wires [5-7], where interaction effects in the wires can be treated non-perturbatively via bosonization. Such systems can exhibit the integer or fractional quantum Hall effect, spin Hall effect, and anomalous Hall effect.

[1] J. Klinovaja and D. Loss, Phys. Rev. B 86, 085408 (2012). [2] J. Klinovaja, P. Stano, A. Yazdani, and D. Loss, Phys. Rev. Lett. 111, 186805 (2013). [3] J. Klinovaja and D. Loss, Phys. Rev. B 90, 045118 (2014). [4] J. Klinovaja, A. Yacoby, and D. Loss, Phys. Rev. B 90, 155447 (2014). [5] J. Klinovaja and D. Loss, Phys. Rev. Lett. 111, 196401 (2013); J. Klinovaja and D. Loss, Eur. Phys. J. B 87, 171 (2014). [6] J. Klinovaja and Y. Tserkovnyak, Phys. Rev. B 90, 115426 (2014). [7] J. Klinovaja, Y. Tserkovnyak, and D. Loss, Phys. Rev. B 91, 085426 (2015).

Invited Talk O 99.5 Fri 11:45 H1

Skyrmions – Topological magnetization solitons for future spintronics — •Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

Ultrathin magnetic films and heterostructures provide a fantastic playground for the stabilization, manipulation and usage of chiral magnetic skyrmions – topological magnetization solitons – magnetic entities described by a micromagnetic energy functional with particle like properties that may open a new vista for spintronics. A crucial quantity for the chiral skyrmion formation is the Dzyaloshinskii-Moriya interaction (DMI), whose presence in thin films could be established in a concerted effort of first-principles theory and spin-polarized scanning tunneling microscopy. It could be shown that the spin-orbit interaction and the structure inversion-asymmetry in these systems result in a DMI that is strong enough to give rise to one- and two-dimensional lattices of chiral spin-textures, chiral domain walls and even single skyrmions. In

retrospect, it is surprising how little is known about the DMI in these metallic systems. In this talk I give insight into the DMI, relating first-principles calculations to different models, discussing the transport properties of electrons *e.g.* the topological (THE) and anomalous (AHE) Hall effect in relation to the spin texture of a skyrmion, and discuss possibilities to tailor the magnetic interactions to enlarge the materials base to stabilize single skyrmions. – I acknowledge fruitful collaborations with D. Crum, J. Bouaziz, B. Dupé, S. Heinze, N. Kiselev, S. Lounis, Y. Mokrousov, A. Nandy, and B. Zimmermann.