Contents

General information

Organizers

- Ferdi Aryasetiawan, University of Lund - Sweden

- Claudio Verdozzi, University of Lund - Sweden

- Martin Stankovski, University of Lund - Sweden

- Zeila Zanolli, RWTH Aachen - Germany

- Nicole Helbig Forschungszentrum Jülich - Germany

- Gabriele D'Avino, Mons University - Belgium

- Michiel van Setten, Université Catholique de Louvain - Belgium

ETSF Steering committee

The ETSF Steering Committee consists of nine elected Research Team Leaders. The current SC members are:

- Prof. Matthieu Verstraete (Université de Liège, Belgium), Chair

- Prof. Rex Godby (University of York, United Kingdom)

- Prof. Andrea Marini (Consiglio Nazionale delle Ricerche, Italy)

- Prof. Giovanni Onida (Università Degli Studi di Milano, Italy)

- Dr. Francesco Sottile (Ecole Polytechnique, Palaiseau, France)

- Prof. Lucia Reining (Ecole Polytechnique Palaiseau, France)

- Prof. Myrta Gruning (Queen's University Belfast, UK)

- Prof. Gian-Marco Rignanese (Catholic University of Louvain, Belgium)

- Prof. Claudio Verdozzi (University of Lund, Sweden)

Support

Workshop Venue

The workshop will be held at *Eden* (in the Political Sciences building) on the days 20-22/9 (Tuesday to Thursday), and at *Palaestra* on Friday the 23/9. These venues are very close to the main university building on the old central campus in the city of Lund. Locations are marked as number 1 (Eden) and 2 (Palaestra) respectively on the map. Coffee breaks and the poster session are hosted just outside the Eden main auditorium, which is located to the right after coming in through the main entrance.

Talks location

The main lecture hall in the *Eden* bulding has a capcity for 140 people and state-of-the art projection and teleconferencing facilities. The same applies for *Palaestra*.

Conference Secretary and local contacts

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Internet Access

Wi-fi is available in all Lund University areas via "eduroam". Individual access is also available via the access details provided with this booklet.

Posters

The posters can be put up from 12:00 on Wednesday the 21st, the day of the poster session. The boards will be situated just outside the main lecture hall. Posters must be taken down by the first coffee break on Friday the 23rd.

Breaks

There will be 30 minute breaks during morning (at 10:15 am) and afternoon (at 3:15 pm) sessions. Coffee, tea, drinks and snacks will be available just outside the conference room. On Thursday 22nd, there will be no afternoon break. The lunch breaks will last for 2 hours, and lunches will be at different restaurants in Lund.

Conference desk

The Conference desk will be located just inside the main entrance to the *Eden* building

Social Program

On Thursday 22nd, there will be a guided tour of the MAX IV Laboratory, a new Synchrotron radiation facility outside Lund. The tour will approximately take 1 hour. Later in the evening (around 7:00 pm), the conference dinner will take place at the restaurant Hurva Gästgivaregård, also outside Lund. Transportation to/from Max IV and Hurva locations will take place by bus/coach. People interested in these events will be asked to confirm they participation during the meeting, where further schedule details will be provided.

Transportation

All conference locations, hotels, recommended restaurants and other places of interests are within a 1 km radius, often closer. Should you need special transportation, the recommended taxi number is: +46-(0)46 121212

For the visit to MAX IV and the conference dinner bus/coach transport will be arranged with further details will be disseminated on that day. The pickup points for bus transport connected to the visit to MAX IV and the conference dinner are marked on the map.

Program

	Monday 19 Registration
13:30	Registration Coffee
14:00	SC and MB
16:00	software meeting
	Tuesday 20 Strongly correlated materials: non-magnetic effects
08:45	Welcome
09:00	Igor Abrikosov - Correlated systems at extreme conditions
09:35	Nicole Helbig - Generalized Pauli constraints in reduced density matrix functional theory
09:55	Daniel Karlsson - Partial Phi-derivability and analytic properties in many-body perturbation theory, and implications for sum rules
10:15	Coffee Break
10:45	Silke Biermann - Electronic structure calculations for correlated materials – A Dynamical Mean Field Theory perspective
11:20	Rex Godby - Exact DFT and TDDFT potentials for correlated electrons in real space
11:40	Michiel van Setten - High-throughput GW: automatization methodologies and large scale validation
12:00	Lunch
14:00	Anders Blom - Commercial vs. academic software: a love-hate story
14:35	Michael Kuhn - Two-component methods in the framework of time-dependent density functional theory
14:55	Nicolas Dardenne - Many body perturbation theory on lead candidates for high-performance organic photovoltaics
15:15	Coffee Break
15:45	Dook van Mechelen - Electronic properties of Mg-Ni-H across the metal-to-insulator transition for industrial hydrogen sensing
16:20	Round Table with industry
17:05	ETSF General meeting
18:05	User Project meeting discussion on how to proceed

	Wednesday 21 Strongly correlated materials: magnetic effects
09:00	Hubert Ebert - Recent extensions to the one-step theory of photoemission
09:35	Thomas Ostler - First Principles Calculation of Curie temperatures and temperature dependence of magnons in magnetic materials
09:55	Hugo Strand - Hund's exchange out of equilibrium
10:15	Coffee Break
10:45	Silvia Picozzi - Relativistic ferroelectrics: a novel class of multifunctional materials
11:20	Alireza Akbari - Magnetic phases in parent compounds of iron-chalcogenides via quasiparticle scattering interference
11:40	David O'Regan - Bandwidth renormalization and satellites in SrVO3 from a minimal DFT+U inspired model
12:00	Lunch
14:00	Pascale Deen - Emergent behaviour and magnetic frustration
14:35	Alexander Yaresko - Direct observation of spin-orbit coupling in iron-based super-conductors
14:55	Zeila Zanolli - Designing new materials for spintronics: the exemplar case of graphene-on-multiferroics
15:15	Coffee Break
15:45	Yaroslav Pavlyukh - Vertex function of homogeneous electron gas: positive definite approximation
16:05	Vojtch Vlcek - Stochastic formulation of the GW approximation
16:25	Thorsten Deilmann - Three-particle correlation from a many-body perspective: Trions in a carbon nanotube
16:45	Poster Session (food and drinks)
20:00	End poster session

	Thursday 22 Spin dynamics and transport
09:00	Gianluca Stefanucci - Should we really give up with DFT in strongly correlated quantum transport?
09:35	Christoph Friedrich - Spin-wave excitations and electron-magnon scattering from many-body perturbation theory
09:55	Alexey Kartsev - Light-induced spin crossover in an ordered single molecular layer
10:15	Coffee Break
10:45	Anna Delin - Spin dynamics and spin-heat interaction
11:20	Miroslav Hopjan - Negative friction in molecular tunnel junctions: the role of electronic correlations
11:40	Stefano Pittalis - U(1)XSU(2) Gauge-Invariance Made Simple for Density Functional Approximations
12:00	Lunch
14:00	Mechthild Enderle - Twisted excitations in low-dimensional quantum magnets
14:35	Nicholas Pike - Coupled Boltzmann Equation Solver: Effects of the Electron-Phonon interaction on the Transport Coefficients
14:55	Gabriele D'Avino - Combining the many-body GW formalism with classical discrete polarizable models: a novel route to the QM/MM description of complex molecular systems
15:15	Ryan McMillan - Projected Equations of Motion (PEOM) Approach to Hybrid Quantum/Classical Dynamics in Composite Materials
15:35	Max Lab Speech: Jesper Andersen (director)
16:00	transfer to Max Lab
16:30	Max Lab Tour
17:30	transfer to Lund
18:00	break
18:30	transfer to dinner
19:00	Workshop Dinner

	Friday 23 Spectroscopy
09:00	Liu Hao Tjeng - Search for new f-electron topological materials
09:35	Emil Boström - Time-resolved spectroscopy at surfaces and adsorbate dynamics: insights from simple model systems
09:55	Matthieu Verstraete - Long-range dispersion forces between molecules subject to attosecond pulses from ab initio calculations
10:15	Coffee Break
10:45	Anders Mikkelsen - Imaging and spectroscopy of Low Dimensional Structures to the Ångström Length and Attosecond Time Scales.
11:20	Barbara Brena - First-principles modelling of the L-edge X-Ray Absorption Spectroscopy of Transition Metal Oxides
11:40	Roman Ovcharenko - X-ray emission and absorption spectra calculation scheme within the traditional DFT and beyond
12:00	Jianqiang Zhou - Recent developments in cumulant approaches to photoemission spectra
12:20	Closing remarks
12:35	Lunch

Abstracts

Oral Contributions

Correlated systems at extreme conditions

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Theoretical simulations of transition metals and their alloys at extreme conditions of ultra-high pressure and temperature generally rely on a picture of non-magnetic wide-band systems with insignificant local correlations. Upon compression, the overlap between localized states increases and so does the bandwidth W, while the local Coulomb repulsion U between those states is screened more efficiently. The reduction of the U/W ratio is used to rationalize the absence of electronic correlations beyond the local or semi-local approximations within the Density Functional Theory (DFT) at high-pressure conditions. We show that this generally accepted picture is incorrect. Carrying out theoretical simulations at the level of Dynamical Mean-Field Theory combined with DFT (DFT+DMFT) [1] coupled to advanced experimental studies of materials at extreme conditions, we show that many-electron effects may have strong influence on the electronic structure and properties of transition metals, their alloys and compounds. Indeed, it is well known that correlation effects are essential for a description of the pressure induced insulator-to-metal transitions (IMT). We illustrate this by considering IMTs in transition metal oxides [2,3]. Moreover, considering hcp Fe and Os, we show that including correlation effects is necessary for the description of the topological changes of the Fermi surface for valence electrons at high pressure, the so-called electronic topological transition (ETT) [4,5]. Considering Fe at the conditions of the Earth's core, we show that DFT+DMFT calculations allow one for better understanding of the Earth's geodynamo [6,7]. Finally, considering Os compressed to over 770 GPa, we discuss the anomaly observed experimentally in the behavior of the unit cells parameters ratio c/a at about 440 GPa. We argue that the anomaly might be related to a new type of electronic transition, the core level crossing (CLC) transition, associated with interactions between the core electrons induced by pressure [5].

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[2] V. Potapkin, L. Dubrovinsky, I. Sergueev, M. Ekholm, I. Kantor, D. Bessas, E. Bykova, V. Prakapenka, R. Hermann, R. Rüffer, V. Cerantola, J. Jönsson, W. Olovsson, S. Mankovsky, H. Ebert, and I. A. Abrikosov, Phys. Rev. B **93**, 201110(R) (2016).

[3] I. Leonov, L. Pourovskii, A. Georges, and I. A. Abrikosov, in manuscript.

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[6] L. V. Pourovskii, T. Miyake, S. I. Simak, A. V. Ruban, L. Dubrovinky, and I. A. Abrikosov, Phys. Rev. B **87**, 115130 (2013).

[7] L. V. Pourovskii, J. Mravlje, A. Georges, S. I. Simak, I. A. Abrikosov, arXiv:1603.02287 [cond-mat.str-el].

Generalized Pauli constraints in reduced density matrix functional theory

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Reduced Density Matrix Functional Theory is a method that relies on the 1-1 correspondence between the many-body ground-state wave function and the first order reduced density matrix (1RDM) and uses the latter as its fundamental variable. The ground state of a system is determined within this approach by minimizing the energy functional with respect to the 1RDM under the constraint that the 1RDM corresponds to a fermionic ensemble (Coleman's conditions). For systems with a non-degenerate ground-state, the minimization of the exact energy functional using the ensemble representability constraints would yield a 1RDM that corresponds to a pure state, i.e. the ground state. As the explicit expression of the energy functional with respect to the 1RDM is unknown, different approximate functionals are employed. For these approximate functionals we found, for several three-electron test cases, that the energy minimization results in occupation numbers that do not satisfy the generalized Pauli constraints (GPC), i.e. the 1RDM does not correspond to a pure state. In principle one can employ the GPC as additional constraints during the energy minimization to ensure that the resulting ground-state 1RDM corresponds to a pure state. However, due to the exponential growth of the number of constraints with the number of particles and the number of natural orbitals in the calculation this is not feasible in practice apart from a few cases of really small systems. Therefore, we discuss the idea of applying the GPC in an approximate way to only the electrons that have occupations smaller than one since in larger systems several natural orbitals become almost fully occupied. These orbitals do not play any role in the question whether the 1RDM corresponds to a pure state or not. Although it is doubtful whether 1RDMs with occupations that are exactly one can correspond to a ground state of a real fermionic system, in many cases this is a sensible approximation that would significantly reduce the amount of GPC to be considered in a RDMFT minimization. We also discuss how the GPC can be extended to

include the spin degrees of freedom and show results for the lowest singlet-triplet excitation energies.

[1] I. Theophilou et al, J. Chem. Phys. **142**, 154108 (2015).
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Partial Φ-derivability and analytic properties in many-body perturbation theory, and implications for sum rules

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A Φ-derivable approximation in many-body perturbation theory guarantees the fulfillment of several conservation laws. We introduce the concept of partial Φ-derivability where only parts of the Φ-functional is dressed with the full Green's function. By various amount of dressing, several commonly used, partially self-consistent, approximations can easily be deduced to either fulfil or violate the continuity equation (particle number conservation). We show that by dressing each loop in Φ consistently, a number conserving approximation is obtained which however does not have to fulfil other conservation laws. Within partially Φ-derivable schemes, and under the additional assumption of correct analytical properties for the Green's function, a general sum rule can be derived, which reduces to the Luttinger-Ward theorem in the case of a homogeneous electron gas, and the Friedel sum rule in the case of the Anderson model. Additional terms in the sum rules are needed if the approximation is not number conserving.

Electronic structure calculations for correlated materials – A Dynamical Mean Field Theory perspective

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Dynamical mean field theory (DMFT), in conjunction with electronic structure techniques such as density functional theory (DFT), has led to tremendous progress in the description of excited state properties of materials with strong electronic Coulomb correlations. The challenge nowadays consists in refining the interface of electronic structure and many-body theory in order to develop quantitatively accurate predictive schemes. In this talk, we focus on recent efforts of incorporating dynamical screening effects into a DMFT-based description of correlated materials [1]. Such effects can stem either from higher energy degrees of freedom that have been integrated out or from nonlocal processes that are effectively backfolded into a local description. This can be conveniently done by combined many-body perturbation theory and dynamical mean field theory ("GW+DMFT") techniques [2]. An analysis of the effects of the different corrections to standard DFT+DMFT schemes leads to new insights also into DFT itself [3, 4].

[1] For a review, see S. Biermann, J. Phys.: Condens. Matter 26 173202 (2014).
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Exact DFT and TDDFT potentials for correlated electrons in real space

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The iDEA code [1] allows investigation of many-electron effects in the exact functionals of ground-state and time-dependent density-functional theory, contributing to the development of new functionals [2] and theories for static and dynamic systems of correlated electrons. Use of a real-space one-dimensional system permits a more realistic description of electron correlation and dynamics than lattice models, yet remains amenable to exact solution of the many-electron Schrödinger equation and reverse-engineering of the electron density to obtain the exact Kohn-Sham (KS) potential. I shall describe our recent investigation of the presence of steps in KS potentials [3], in which we find that steps occur at points in the electron density where there is a change in the 'local effective ionisation energy' of the electrons. Other studies using iDEA shed light on strong correlation in the homogeneous electron gas [4] and the relationship between many-body perturbation theory and DFT [5].

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[5] L. Talirz, J. Wetherell, M.J.P. Hodgson and R.W. Godby, unpublished.

High-throughtput GW: automatization methodologies and large scale validation

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Many technologically important material properties directly relate to their electronic structure. Computational screening studies searching for new materials with specific properties hence rely on methods that accurately predict electronic structure and do so in automatic manner. For solids the GW-method is currently one of the most reliable *ab initio* approaches to predict electronic structure. It is mostly used to perturbatively correct density functional theory results from fundamental shortcomings and errors introduced by the approximate exchange correlation functional. It is however computationally demanding and requires much expertise to perform accurately. For its applications in high throughput screenings hence sophisticated algorithms for setting up the calculations and determining convergence are needed. In this work we develop such a method and, as a first application, use it to validate the accuracy of G_0W_0 using the PBE starting point (G_0W_0@PBE) and the Godby-Needs plasmon pole model on a set of about 100 solids. The automatic convergence screening utilized in this works provides valuable insights, e.g., correlations between computational parameters, that can be used to further improve the automatization of GW calculations. The large scale validation of G_0W_0@PBE shows a correlation between the PBE and the G_0W_0@PBE gaps that is much stronger than that between GW and experimental gaps. With this work we hence show that GW can be made automatic but that for accurate predictive results for a broad class of materials an improved starting point or form of self-consistency is necessary.

Commercial vs. academic software: a love-hate story

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QuantumWise A/S

For over 13 years, QuantumWise has worked on developing commercial software tools for atomic-scale simulations. During this time we have collaborated with academic groups on several levels, involving both pure research into new algorithms and methods, co-implementation of libraries, and integration of existing code of various types. This has given us a lot of insight into the dynamics between academic and commercial software, how they can co-exist, and what works and what doesn't both from the perspective of the distributor (the commercial partner) and the end-user. In my presentation I will explore this relationship, touching on topics like code quality, licensing models, pricing, open/closed source, and the roles of professional software manufacturers vs. that of scientists. In addition you will learn about how our tools can be used for atomic-scale simulations within materials science and nanoelectronics, and in particular how our platform allows users to set up calculations with almost any software packages (like VASP, Abinit, QuantumEspresso, LAMMPS) and analyzing the output results.

Two-component methods in the framework of time-dependent density functional theory

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This talk reports on the efficient implementation and application of a two-component variant of time-dependent density functional theory (TDDFT) [1] that accounts for spin-orbit effects on excitations of closed-shell molecules by employing a noncollinear exchange-correlation functional in combination with relativistic pseudopotentials. The implementation was done in the TURBOMOLE program package, which utilizes localized Gaussian basis functions. Based on this implementation a two-component extension of the G_0W_0 method [2] was also implemented, which accounts for spin-orbit effects on one-electron energies of isolated molecular systems. The efficiency of our two-component TDDFT implementation is demonstrated by calculation of the optical absorption spectrum of the large ligand-protected gold cluster $Au_{25}(SCH_3)_{18}^-$. It is shown that the double peak structure in the measured optical absorption spectrum, which has not been understood so far, can be traced back to spin-orbit coupling. Furthermore, we apply our two-component TDDFT implementation to the calculation of phosphorescence in Iridium compounds relevant for organic light-emitting diodes (OLEDs). In general, a short lifetime of the excited triplet state is advantageous for a good luminous efficiency of OLEDs. Our predictions for those lifetimes are in good agreement with the experiment.

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[2] M. J. van Setten, F. Weigend and F. Evers, J. Chem. Theory Comput. **9**, 232 (2013).

Many body perturbation theory on lead candidates for high-performance organic photovoltaics

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In organic photovoltaic (OPV) cells, the photocurrent generation efficiency depends critically on charge–separation (CS) of the electron-hole (exciton) at the interface between electron donor and acceptor phases. This CS process depends on charge transfer (CT) effects taking place at the donor–acceptor interface. In order to theoretically devise new OPV cells with high efficiency, it is thus important to describe these CT effects adequately. In this framework, the Green's function based many-body perturbation theory (MBPT) constitutes a choice tool for computing the electronic and optical properties of materials [1]. Since the mid-80s, this approach has proven very accurate for extended semiconductors. In particular, the so-called GW/BSE formalism correctly reproduces experimental electronic and optical band gap in many studied systems. Recently, an efficient "auxiliary Gaussian basis" implementation of the GW/BSE formalism (the Fiesta code [2]) has been developed allowing to treat molecular systems consisting of up to a few hundred atoms.
The present project aims at studying the electronic and optical properties of the interface between various theoretically designed donors and an acceptor (fullerene C60) using the Fiesta code. Tens of thousands of molecules have been already tested in a multiple-step screening within the Harvard Clean Energy Project (CEP) [3], leading to a ranking of potential candidates for efficient organic photovoltaics. However, the calculations have been performed relying on density-functional theory which is known to underestimate the band gap and not to describe electron-hole interaction and CT effects correctly. Here, we focused on the top 21 donor molecules from the CEP ranking. In a first step, we computed the electronic and optical properties for the donor alone. In a second step, we considered the complete fullerene-donor complexes and computed highly accurate band gaps, exciton binding and charge-transfer energies. The Harvard group computed the equilibrium geometries of the complexes and the UCL team carried out the corresponding GW/BSE calculations. From these results, we were able to evaluate possible efficiency loss pathways.

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G. Onida, L. Reining, A. Rubio, Rev. Mod. Phys., 74, 601, 2002.

[2] Charge-transfer excitations in molecular donor-acceptor complexes within the many-body Bethe-Salpeter approachX. Blase and C. Attaccalite, Applied Physics Letters 99, 171909, 2011.

[3] Lead candidates for high-performance organic photovoltaics from high-throughput quantum chemistry – the Harvard Clean Energy Project, Johannes Hachmann et al., Energy Environ. Sci., 7, 698-704, 2014.

Electronic properties of Mg-Ni-H across the metal-to-insulator transition for industrial hydrogen sensing

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Optical hydrogen sensors have a promising future in a society where hydrogen detection becomes increasingly essential. The traditional use of Pd as sensing material is disadvantaged by its small optical contrast and low sensitivity. A solution is found by transition metal hydrides that cross a metal-to-insulator transition upon hydrogenation. Since a typical hydrogen sensor operates in a continuous hydrogen pressure range, knowledge of the optical properties in the vicinity of the metal-to-insulator transition is crucial. Here we present an optical spectroscopy study on Mg-Ni-H where we investigate the approach towards the insulating state. Upon increasing the hydrogen content, the infrared conductivity demonstrates a strongly decreasing intraband peak and upcoming mid-infrared spectral weight. DFT calculations of hydrogen deficient Mg_2NiH_x indicate that for hydrogen vacancy concentrations between 0.25 and 2 per unit cell, states appear in the original gap of Mg_2NiH_4. Transitions involving these states cause significant mid-infrared spectral weight, in agreement with the experiment. In this talk, we put forward how the observed optical properties in relationship with DFT models and the proposed strongly correlated mechanism of the metal-to-insulator transition are of importance for industrial optical hydrogen sensing.

Recent extensions to the one-step theory of photoemission

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During the last decades the one step model of photo-emission was extended in various ways. An important step was the introduction of the Coherent Potential Approximation (CPA) that led to a very reliable description of angle resolved photo emission spectroscopy (ARPES) of transition metal alloys. Making use of the alloy analogy model the CPA has been exploited as well to deal with thermal lattice vibrations treated in a quasi-static manner. This scheme has recently been complemented by a corresponding description of thermal spin fluctuations that are of crucial importance for the properties of magnetic materials at finite temperatures. The second part of the talk will be devoted to the extension of the one-step model to deal with pump-probe photo emission. The approach is based on a general treatment of the photo emission process using the Keldysh formalism for the lesser Green function to describe the real-time evolution of the electronic degrees of freedom in the initial state after a strong pump pulse that drives the system out of equilibrium. The final state is represented by a time-reversed low energy electron diffraction (LEED) state. The formalism allows for a quantitative calculation of the time-dependent photo current that results from core or valence-band excitations, and is applicable to simple metals or more complex materials like topological insulators. So far the scheme has been implemented to deal with two-photon photo emission (2PPE) where both the pump-pulse and the probe pulse are weak in intensity. As a first application results for 2PPE spectra of Ag(100) are presented, where the first image state serves as an intermediate state to probe the occupied band structure below the Fermi level. Application of the approach to more complex situations as well as its application to other types of spectroscopy will be discussed.

First Principles Calculation of Curie temperatures and temperature dependence of magnons in magnetic materials

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Magnons are the elementary magnetic excitations in ordered solids. Understanding such collective excitations is important for a number of technologically relevant fields, such as, magnonics [1] or spin caloritronics [2]. The central interactions in spin caloritronics are the couplings of phonons with electrons and spin degrees of freedom. Furthermore, understanding the effects of temperature on the phonon and spin degrees of freedom adds a further complexity. In the present work we have developed a multiscale model of ferromagnetic materials and demonstrate the effect of temperature dependent phonon displacements on the magnons spectra. Our results show that the for Fe and Ni the effect of phonon displacements acts to reduce the Curie temperature, whereas for Permalloy the opposite is true due to an increased long-ranged exchange interaction. This increased exchange interaction results in an increasing spin-wave stiffness with increasing temperature, overcoming the usual decrease due to magnon softening. To determine the effects of increasing the phonon temperature we have developed a multiscale model whereby we begin by calculating the thermal displacement of phonons, $\sqrt{\langle u^2(T) \rangle}$, calculated using the phonopy software package [3] using electronic ground state and phonon properties determined using the ABINIT software package [4]. Then the exchange constants are determined using the SPRKKR package [5]. Finally, we use linear spin wave theory to determine the effect of the phonon temperature on the exchange alone, demonstrating an increasing frequency of the acoustic magnon branch. We take into account the thermal effects of the magnetic system through the use of the atomistic spin dynamics approach. Magnon softening due to thermal effects demonstrates a more modest increase in the exchange stiffness (over the purely phononic effect), however, an overall increase is still observed.

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Hund's exchange out of equilibrium

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The non-equilibrium properties of strongly correlated materials is a very active field of research. Experimentally the field of optical pump-probe setups is pushing the boundaries of observable non-equilibrium quantum many-body effects. Theoretically a promising method is real-time dynamical mean-field theory which has been applied successfully to both the fermionic and bosonic Hubbard models. While the majority of previous theoretical studies has been restricted to the single-band Hubbard model, there are a plethora of many-body effects that emerges only in multi-orbital setups. A prime example is the spin-freezing effect that is driven by fermionic inter-orbital Hund's exchange. Using real-time dynamical mean-field theory and first- and second-order strong coupling expansion impurity solvers, we here report calculations on the non-equilibrium dynamics of the canonical model for strongly correlated Hund's metals, the two band Hubbard model with local density-density and Hund's exchange interaction.

Relativistic ferroelectrics: a novel class of multifunctional materials

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The discovery of novel properties, effects or microscopic mechanisms in modern materials science is often driven by the quest for the coexistence and/or coupling of several functional properties into a single compound. Within this framework, by exploiting the interplay between spin and dipolar degrees of freedom via spin-orbit coupling in ferroelectric semiconductors, I will focus on the tight link between k-dependent spin-splitting in the electronic structure, spin-texture and electric polarization. Based on density functional simulations, I will show our theoretical predictions of a giant Rashba spin-splitting in "bulk" GeTe[1], prototype of novel multifunctional materials - labeled as Ferro-Electric Rashba Semi-Conductors (FERSC)[2] - where the chirality of the spin texture is one-to-one linked to polarization. As the latter can be induced/controlled/switched via an electric field in a non-volatile way, the integration of semiconductor spintronics with ferroelectricity is envisaged. In the second part of the talk, the connection between ferroelectricity and spin-degrees of freedom will be discussed by providing examples from different materials classes (oxides heterostructures,[3] halides perovskites,[4] chalcogenides, etc), all of them showing strong relativistic effects.

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Magnetic phases in parent compounds of iron-chalcogenides via quasiparticle scattering interference

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One of the biggest mysteries of the Fe-based superconductors is the striking difference between the magnetic phase of the pnictide and chalcogenide compounds. The parent compounds of the Fe-pnictide superconductors show a magnetic state with a $(\pi,0)$ spin density wave (SDW) vector which gives way to superconductivity upon doping and/or application of pressure. The Fermi surfaces in both the pnictides and chalcogenides in general show common features such as hole pockets at the Γ-point and electron pockets at the X and Y points of the Brillouin zone. These pockets are well nested at the wave vector of $(\pi,0)$ or $(0,\pi)$. This is also the wave vector of the SDW, and hence band nesting is commonly accepted as the mechanism of the SDW in the pnictide compounds. However, the chalcogenides show a completely different magnetic structure, with a SDW wave vector of $(\pi/2,\pi/2)$ for zero or low doping, forming the so-called double-striped (DS) phase and hence the origin of the SDW in the chalcogenides cannot be explained by the nesting of the hole and electron bands. The origin of the SDW in the chalcogenides is still under hot debate. We employ a five-orbital tight-binding model to develop the mean-field solution for various possible spin density wave states in the iron-chalcogenides. The quasiparticle interference (QPI) technique is applied to detect signatures of these states due to scatterings arising from non-magnetic impurities. Apart from the experimentally observed double-striped structure with ordering vector $(\pi/2,\pi/2)$, the QPI method is investigated for the extended-stripe as well as the orthogonal double-stripe phase. We discuss QPI as a possible tool to detect and classify various magnetic structures with different electronic structure reconstruction within the framework of the $Fe_{1+y}Te$ compound.

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Bandwidth renormalization and satellites in SrVO$_3$ from a minimal DFT+U inspired model

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In contemporary first-principles atomistic simulation based on DFT, the augmentation of approximate exchange-correlation functionals with spatially or energetically localized corrections, such as DFT+U, is a successful approach for improving its applicability to strongly interacting systems. Electronic screening is a dynamical process, and since the Hubbard U parameter, in particular, is a measure of the screened Coulomb interaction, its frequency-dependent generalisation for the dynamical regime is possible. We introduce a conceptually pragmatic and computationally straightforward method, named DFT+$U(\omega)$, for calculating and incorporating strong dynamical screening effects in spectroscopic calculations based on Kohn-Sham DFT. Our method is designed to be a minimal dynamical extension of DFT+U, one in which computing approximate dynamical Hubbard U functions only requires functionality that is widely available. We demonstrate our effective plasmon fitting and self-energy approximation scheme for DFT+$U(\omega)$, which enables the resulting low-energy dynamical model to be solved at the G_0W_0 level, and beyond, efficiently and effectively.

Emergent behaviour and magnetic frustration.

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Frustrated magnetic materials are promising candidates for new states because lattice geometry suppresses conventional magnetic dipole order. Frustration thus drives novel emergent states. Classical spins on the 3D triangular hyperkagome lattice have long been considered ideal for novel states yet have provided few examples. $Gd_3Ga_5O_{12}$ is the canonical frustrated magnet since the compound does not order via the pervasive "order by disorder" mechanism down to the lowest temperatures probed, 25 mK [1 and ref. therein]. Short-range correlations, determined via neutron diffraction, have long been assumed to originate from near neighbour short-range interactions [1]. However in recent work an emergent spin state of decagon looped structures at the lowest temperatures has been uncovered [2,3]. These emergent decagon spin loops remain dominant when attempting to polarise the spin structure by a large applied magnetic field [4]. Neutron inelastic scattering shows a dominant contribution at large momentum transfers from a band of almost dispersionless excitations that correspond to the spin waves localized on ten site rings, expected on the basis of nearest neighbor exchange interaction [4]. These result illustrate the richness and diversity that arise from frustrated exchange on the three-dimensional hyperkagome lattice

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Direct observation of spin-orbit coupling in iron-based superconductors

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Spin-orbit coupling is a fundamental interaction in solids that can induce a broad range of unusual physical properties, from topologically non-trivial insulating states to unconventional pairing in superconductors. In iron-based superconductors its role has, so far, not been considered of primary importance, with models based on spin- or orbital fluctuations pairing being used most widely. Comparing angle-resolved photoemission spectroscopy results to results of relativistic band structure calculations, we find a sizable spin-orbit splitting in all the main members of the iron-based superconductors [1]. We demonstrate that in most cases its impact on the low-energy electronic structure and details of the Fermi surface topology is stronger than that of possible nematic ordering. The largest pairing gap is supported exactly by Fermi surfaces affected by spin-orbit coupling, implying a possible relation between this interaction and the mechanism of high-temperature superconductivity.

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Designing new materials for spintronics: the exemplar case of graphene-on-multiferroics

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Graphene and magnetoelectric multiferroics are promising materials for spintronic devices with high performance and low energy consumption. A very long spin diffusion length and high carrier mobility make graphene attractive for spintronics. The coupling between ferroelectricity and magnetism, which characterises magnetoelectrics, opens the way towards unique device architectures. In this work [1], we combine the features of both materials by investigating the interface between graphene and $BaMnO_3$, a magnetoelectric multiferroic. We show that electron charge is transferred across the interface and magnetization is induced in the graphene sheet due to the strong interaction between C and Mn. Depending on the relative orientation of graphene and $BaMnO_3$, a quasi-half-metal or a magnetic semiconductor can be obtained. A remarkably large proximity induced spin splitting of the Dirac cones ($\sim$300 meV) is achieved. We also show how doping with acceptors can make the high-mobility region of the electronic bands experimentally accessible. This suggests a series of possible applications in spintronics (e.g. spin filters, spin injectors) for hybrid organic-multiferroic materials and reveals hybrid organic-multiferroics as a new class of materials that may exhibit exotic phenomena such as the quantum anomalous Hall effect and a Rashba spin-orbit induced topological gap.

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Vertex function of homogeneous electron gas: positive definite approximation

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We present a systematic study of the vertex function correction in homogeneous electron gas at metallic densities. Contrary to a popular belief the vertex function not only provides corrections to the well known plasmon or particle-hole pair scatterings, but also gives rise to new physical processes such as generation of two plasmon excitations or the transformation of the initial one-particle state into a two-particles-one-hole state. Using a merger of the many-body perturbation and scattering theories, which is a distinct feature of our method, it is shown that additional scattering channels are responsible for the bandwidth reduction (as observed in photoemission experiments on bulk sodium), appearance of the secondary plasmonic satellite below the Fermi level and lead to a substantial modification of the electron spectral function.

Stochastic formulation of the GW approximation

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We present formalism of the stochastic GW method discussing its convergence properties, scaling with system size and its computational advantages over deterministic approaches. We demonstrate the method on calculations of ionization potentials and electron affinities of large Si nanocrystals and we further use it to investigate the size and dimensionality dependence of the quasiparticle energy in polythiophene: We compare results of isolated chains (1D) with those of stacked polythiophene chains (2D) for systems with 1500 valence electrons. We demonstrate the practical calculations of the self-energies and show that with increasing system size the approach becomes effectively less expensive leading to approximately linear scaling of the algorithm.

Three-particle correlation from a many-body perspective: Trions in a carbon nanotube

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Trion states of three correlated particles (e.g., two electrons and one hole) are essential to understand the optical spectra of doped or gated nanostructures, like carbon nanotubes or transition-metal dichalcogenides. We develop a theoretical many-body description for such correlated states using an ab-initio approach [1]. It can be regarded as an extension of the widely used GW method and Bethe-Salpeter equation, thus allowing for a direct comparison with excitons. We apply this method to a semiconducting (8,0) carbon nanotube, and find that the lowest optically active trions are red-shifted by ∼130 meV compared to the excitons, confirming experimental findings for similar tubes. Moreover, our method provides detailed insights in the physical nature of trion states. In the prototypical carbon nanotube we find a variety of different excitations, discuss the spectra, energy compositions, and correlated wave functions.

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Should we really give up with DFT in strongly correlated quantum transport?

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Density functional theory (DFT) is certainly not the first method which comes to mind to tackle quantum transport in the strongly correlated regime. Nevertheless, today we have a rigorous DFT-like approach and an accurate exchange-correlation (xc) potential to reproduce the I-V characteristic of the Anderson model, a hallmark of strong correlation, in a wide range of temperatures, gates and biases. In this talk I retrace the steps [1-4] that led us to the current understanding of the problem and discuss some general features of the xc potential to perform ab-initio calculations on strongly correlated nanoscale junctions.

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Spin-wave excitations and electron-magnon scattering from many-body perturbation theory

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Spin excitations form a fundamental class of excitations in magnetic materials. We study the magnetic excitations of bulk Fe, Co, and Ni within the framework of many-body perturbation theory (MBPT) as implemented in the full-potential linearized augmented plane-wave (FLAPW) method. Starting from the *GW* approximation we obtain a Bethe-Salpeter equation for the magnetic susceptibility treating single-particle Stoner excitations and magnons on the same footing. At high energies the spin waves are heavily damped due to the coupling to single-particle Stoner excitations. The obtained results are in good agreement with available experimental data. 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, leading to a substantial improvement of the Goldstone-mode condition. As a cheap alternative, we discuss a correction scheme that involves an adjustment of the KS exchange splitting. The new exchange splittings turn out to be closer to experiment. Finally, we employ the solution of the Bethe-Salpeter equation to construct a self-energy that describes the scattering of electrons and magnons. We show first results.

Light-induced spin crossover in an ordered single molecular layer

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Spin crossover molecules show the unique ability to switch between two spin-states when submitted to external stimuli such as temperature, light or voltage. If controlled at the molecular scale, such switches would be of great interest for the development of genuine molecular devices in spintronics, sensing and for nanomechanics. Unfortunately, up to now, little is known on the behavior of spin-crossover molecules organized in two dimensions and their ability to show cooperative transformation. In this work we demonstrate that the combination of scanning tunneling microscopy measurements and *ab initio* calculations allows discriminating unambiguously between both states by local vibrational spectroscopy. We also show that a single layer of spin-crossover molecules in contact with a metallic surface displays light-induced collective processes between two ordered mixed spin-state phases with two distinct time scales dynamics. These results open a way to molecular scale control of two-dimensional spin crossover layers. This work was partly supported by the Russian Foundation for Basic Research, research project No. 16-32-00157 mol_a.

Spin dynamics and spin-heat interaction

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I will present some recent results involving both atomistic and classical spin-dynamics simulations (based on first-principles calculations). These methods can be used to investigate theoretically a range of spin-based phenomena, such as Gilbert damping and spin stiffness. [1,2] Recently, we have turned some focus toward spincaloritronic phenomena, i.e. the interaction between spin and heat. Specifically, we have studied energy and magnetization transport in oscillator trilayers and networks. In the presence of a thermal gradient, we find a rectification of the flows at certain conditions. Our model also predicts that energy and magnetization in certain situations may flow between two sources with the same temperature and chemical potential. This latter effect can be compared to the well-known dc Josephson effect in superconductors. [3,4]

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Negative friction in molecular tunnel junctions: the role of electronic correlations

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The force exerted by the electrons on the nuclei of a current-carrying molecular junction can be manipulated to engineer nanoscale mechanical systems. It has been reported in the literature that, under general nonequilibrium conditions, the friction coefficient of the nuclear motion can be negative, and responsible for Van der Pol oscillations of the nuclear coordinates. So far, nuclear forces in molecular motors have been investigated only within an independent-electron framework. In this work we extend the treatment to include the effect of electron-electron interactions. Using steady-state nonequilibrium Greens functions, we include the interactions within an adiabatic Ehrenfest scheme for the nuclei, which permits an analytical description of the non-conservative forces. An important result of our work is a generalized formula of the friction coefficient, with a correction due to the correlation self-energy. As a general trend, we observe a suppression of the negative friction region with increasing interactions (included at the level of 2nd-born and t-matrix approximations). We also present preliminary results for a full time-dependent Kadanoff-Baym dynamics in the Ehrenfest approximation for the nuclei when high frequency fields are applied, and discuss how the suppression of negative friction affects Van der Pol-type oscillations of the nuclear coordinates.

U(1)×SU(2) Gauge-Invariance Made Simple for Density Functional Approximations

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A non-relativistic density-functional approach that includes spin-orbit couplings self-consistently is an appealing framework to develop a unified first-principles computational approach for non-collinear magnetism, spintronics, and spinorbitronics. The basic variables of this framework include the (paramagnetic) particle- and spin-currents besides the particle- and spin-densities and the corresponding exchange-correlation (xc) energy functional is invariant under local U(1)×SU(2)-gauge transformations. The xc-energy functional must be approximated to enable practical applications but, contrary to the case of standard DFT, finding simple building blocks suited to deal with realistic atomistic inhomogeneities has been a long-standing challenge. Here, we propose a non-empirical resolution based on the analysis of the short range-behavior of the two-body reduced density matrix and related quantities. Novel exchange-correlation approximations and prototypical applications may also be discussed.

Twisted excitations in low-dimensional quantum magnets

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Many magnetic materials are well described by classical approximations. When conventional magnets are cooled down, their atomic magnetic moments order into a periodic pattern. In quantum magnets, however, the atomic magnetic moments seem to disappear when cooled down close to absolute zero temperature, in spite of their interaction. Here, classical approximations dealing with local moments break down and the collective behavior of the interacting assembly requires a description in terms of a many-body quantum mechanical wave function. While the ground state wave function is usually inaccessible to experimental investigation, its character is nevertheless evidenced in unusual collective excitations which can be probed by inelastic neutron scattering. We present neutron scattering evidence for collective quantum excitations in materials where the magnetic interaction dominates in one or two spatial dimensions.

Coupled Boltzmann Equation Solver: Effects of the Electron-Phonon interaction on the Transport Coefficients

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Recent experimental and theoretical calculations point to a complex interplay between the electron and phonon baths in a wide variety of materials [1,2]. We propose a method of coupling the Boltzmann equations for the electron and phonon baths within the relaxation time approximation which we use to calculate the thermoelectric transport coefficients. Our model for the coupled Boltzmann Equation solver includes analytic models, including $\mathbf{k} \cdot \mathbf{p}$ Hamiltonians and tight-binding Hamiltonians, for both the electron and phonon energies and analytic models for the electron and phonon relaxation mechanisms. From these calculations we hope to better understand the role and interplay of electron-phonon and phonon-phonon interactions on the thermoelectric transport coefficients.

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Combining the many-body GW formalism with classical discrete polarizable models: a novel route to the QM/MM description of complex molecular systems

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Hybrid quantum mechanics/molecular mechanics (QM/MM) approaches are invaluable tools for the theoretical study of complex supramolecular systems of interests in chemistry, biology and materials science. We will report on our original QM/MM scheme merging the many-body Green's function GW formalism with accurate classical polarizable models of atomistic resolution.[1,2] We will first provide an overview of our approach to the merging of QM and classical polarizabilities within the framework of the Gaussian basis GW implementation of the Fiesta code,[3] and then present its application to paradigmatic case of the transport gap of the pentacene crystal, for which we obtain an excellent agreement with reference bulk GW calculations. We further investigate the evolution of the polarization energy of pentacene from the bulk to the surface, where this quantity is actually probed experimentally, and prove that the gap is insensitive to the QM/MM partitioning as a result of the mutual compensation of quantum and classical polarizabilities.[4] The proposed hybrid method offers an attractive strategy to compute the full spectrum of charged excitations in complex molecular environments, accounting on equal footing for intermolecular charge transfer, orbital hybridization, and for the screening contributions originating both from the QM and MM subsystems.

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Projected Equations of Motion (PEOM) Approach to Hybrid Quantum/Classical Dynamics in Composite Materials

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TDDFT and Green's function approaches have become standard in the numerical simulation of spectroscopic phenomena in a wide variety of materials. The computational requirements of such calculations grow with the size of the simulated system. For composite systems one often uses hybrid methods, treating the constituent subsystems using different levels of theory where treating the entire system using the same theory would be computationally impractical. In this presentation, we introduce a hybrid method (PEOM) which describes the dynamics of the larger system classically whilst retaining a fully quantum mechanical description of the smaller system. As a testbed, we look at two composites: a quantum dot-metal nanoparticle hybrid and a system of MoS2/Graphene monolayers. In the first case, we compare the results of the PEOM method with analytical results based on the rotating wave approximation. In the second case we compare the method with the standard super-cell approach which uses linear response TDDFT. We then go on to examine MoS2 on a gold substrate where excitonic effects are important [1] using a real time Bethe-Salpeter equation (BSE) [2] coupled with the PEOM. In this case, a super-cell approach cannot be used due to the computational demand of the BSE.

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Search for new f-electron topological materials

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The interplay of strong spin-orbit coupling and electron-electron correlations in f-electron containing intermetallic systems have recently been shown to allow for the emergence of topologically nontrivial surface bands, thereby bringing into existence the new field of "strongly correlated topological insulators". Using a minimum model consisting of localized f-electrons and dispersive conduction electrons with opposite parity, it has been inferred that f-electron systems with cubic and tetragonal symmetries will open both hybridization plus insulating gaps and host topologically protected metallic surface states, if the ground state multiplet is Γ 8 and Γ 6 , respectively [1,2,3,4]. Motivated by this theory, we will present two candidate materials: $CeRu_4Sn_6$ [5] and SmO [6]. We will discuss the electronic structure of these materials in detail using both synchrotron-based spectroscopic data and parametrized band structure calculations.

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Work done in collaboration with A. Severing[1] , D. Kasinathan[2] , M.W. Haverkort[2]
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Time-resolved spectroscopy at surfaces and adsorbate dynamics: insights from simple model systems

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The development of ultrafast laser technologies has provided a possibility to measure and control electronic behavior in atomic and molecular gases, close to its natural time-scale of a few attoseconds. Many ultrafast processes of technological importance however depends crucially on the atom-surface interaction, e.g. laser induced photocatalysis, which makes them much more challenging to investigate both theoretically and experimentally.

In response to these challenges we introduce a model of pump-probe real-time dynamics of surface systems (Phys. Rev. B 93, 195416), aimed to provide a description on equal footing of several competing time-scales (electron interactions, core-hole relaxation, plasmon screening and anharmonic nuclear dynamics). For finite-size realisations of our model, we use the exact many-body time evolution and a time-dependent DFT description to analyze the transient and longer time desorption dynamics. In this context, we address the role played by the structure of the external fields, e.g. how multiple-pulse protocols of different duration and intensity impact desorption in some prototypical experiments.

To extend our analysis beyond finite-size systems, we introduce two main approximations: i) We use the semi-classical mean-field (Ehrenfest) approximation to describe the nuclear dynamics, and ii) we treat electron interactions within many-body perturbation theory using the non-equilibrium Green's function method, NEGF (J. Phys. Conf. Ser., 696, 012007). A gradual introduction of these approximations allows us to assess the validity of each approach by using the exact results as a benchmark, but also to understand how the finite size affects the results of the exact solution. Here, the effect of a semi-infinite substrate is considered using an embedding self-energy scheme. Finally, we present results for non-adiabatic charge transfer dynamics in donor-acceptor complexes (work in progress).

While based on model systems and/or preliminary in character, our results clearly illustrate the large potential of NEGF to investigate the non-equilibrium dynamics of material surfaces subject to ultrafast laser fields.

Long-range dispersion forces between molecules subject to attosecond pulses from ab initio calculations

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The London-van der Waals dispersion forces arising from instantaneously induced dipoles in molecules are a key ingredient in a wide range of phenomena in physics, chemistry, and biology. Therefore, the ability to control and manipulate dispersion forces between atoms and molecules is of great importance. Because those dispersion interactions depend crucially on the electronic properties of the molecular systems, a simple route to achieve this would consist in manipulating their electronic states. The recent development of ultra-short optical pulses has given researchers unprecedented control over the electronic degrees of freedom. These pulses, tailored in their frequency and envelope, allow the generation of a strongly out of equilibrium population of electronic states. We show how the Hamacker constants characterizing the London-van der Waals interaction between two molecules subject to an optical pulse can be calculated using time-dependent density functional theory (TD-DFT) or standard quantum chemistry methods and present several test cases of molecules subjected to IR and UV attosecond pulses.

Imaging and spectroscopy of Low Dimensional Structures to the Ångström Length and Attosecond Time Scales.

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We combine microscopy/spectroscopy to the atomic scale, ultra fast laser technology, synchrotron sources and advanced nanoscale device manufacturing. This allow development and use of a new imaging techniques with potential for orders of magnitude better resolution in both time and space for direct studies of materials and devices confined in one or more dimensions - even during operation. Two main themes will be covered: Firstly, we combine the femtosecond and attosecond time resolution of advanced lasers with the nanoscale spatial resolution of PhotoEmission Electron Microscopy (PEEM). Using 5.5 femtosecond laser pulses with a central energy around 1.6 eV in an interferometric time-resolved PEEM setup, we observe differences in near-field enhancement inside a variety of nanostructures already within the first few optical cycles[1,2]. We demonstrate imaging using <100 attosecond laser pulses with central energies between 30-100eV in combination with PEEM (attoPEEM)[3,4] and outline the pathway for using such pulses for direct investigations of photon excitations with sub-femtosecond precision. The combination of advanced lasers and PEEM allows for very sensitive measurements of plasmonics fields, surface chemistry and pump-probe experiments on ultrafast time scales - all in the same picture. Secondly, we have developed and used scanning probe microscopy and high brightness synchrotron based microscopy to determine structure, chemistry and physical properties of III-V semiconductor nanowires. We have developed novel methods to directly image surfaces both inside, outside and topside of nanowires down to the single atom level[5,6]. We have now extended this too direct imaging of nanowire devices in operation[7,8] and have now found that real atomic resolution can be achieved during operation. Using our rather diverse toolbox we can obtain a real understanding of the connections between structure, growth and function of these nanowires.

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First-principles modelling of the L-edge X-Ray Absorption Spectroscopy of Transition Metal Oxides

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We present a novel computational scheme for the calculation of the L2,3 edges x-ray absorption spectra (XAS) based on the combination of Density Functional Theory + Dynamical Mean Field theory [1](DFT+DMFT) and Multiplet Ligand Field Theory (MLFT)[2]. The L edge x-ray absorption spectroscopy implies the excitation of core 2p electrons into valence 3d levels. In materials like transition metal oxides and in molecules with transition metal centers, the highly correlated 3d electrons are responsible for the magnetic properties as well as for many-body effects like Kondo resonances and superconductivity. The theoretical treatment of these electronic excitations poses a big challenge for ab initio methods. In addition to the intrinsic difficulty in describing the strong correlation of the d electrons, complex effects like the ligand field generated by the neighboring atoms, the multiplet structure associated with the spin-orbit coupling in 2p and 3d shells as well as the final state with a 2p hole have necessarily to be included. In the developed method, the impurity and bath states of the MLFT are constructed from ab-initio DFT calculations. The XAS Hamiltonian accounts for the 2p to 3d excitations, and is obtained through a multiplet approach, where correlation effects are included according to the Single-Impurity Anderson Model[3]. The transition probabilities are computed within the dipole approximation. In the present work, this method has been applied to the calculations of L-edge spectra of a series of transition metal oxides, such as MnO, FeO, CoO, NiO, resulting in a very good agreement with the experimental data.

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X-ray emission and absorption spectra calculation scheme within the traditional DFT and beyond

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Here we present the computational scheme for X-ray emission and absorption spectra of solids taking into account many electron effects [1]. In this approach the crystal electronic initial and final states are calculated using VASP code with the pane wave basis set. It is well known that within the DFT it is possible to reproduce X-ray K and $L_{2,3}$ emission/absorption spectra for some materials, for example, for magnesium or zinc oxides. However, already for simple metals the one electron approach is unable to give even qualitatively good agreement between the calculated and measured $L_{2,3}$ bands because of the many-electrons effects accompanying the X-ray electron transition. Some of such effects, namely the electron-hole interaction, is possible to treat *ab initio*; the others, like Auger decay in the conduction band, demand at least one fitting parameter. Our implementation allows one to perform such kind of calculations, taking into account the many-electron effects, for any system of interest. Moreover, it provides some useful tools, like spatial decomposition of X-ray intensity into intra-atomic contributions as well as contributions transferred from the ligand atoms, which are closely connected to the charge localisation and redistribution during radiative transition. The code was tested on a number of systems of different nature: from metal oxides [2] to simple metals [3] and graphene [4]. Excellent agreement between the computed and measured spectra was found for all studied cases. [1] ELSA, Version 2.0; https://sites.google.com/site/elsaspectroscopy. [2] R. Ovcharenko et al, Optics and Spectroscopy, **111** p. 940 (2011) [3] R. Ovcharenko et al, Phys. Chem. Chem. Phys. **15**, 6749 (2013) [4] E. Voloshina et al, J. Chem. Phys. **138**, 154706 (2013)

Recent developments in cumulant approaches to photoemission spectra

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Green's function (GF) methods have been very successful for describing one- and two-particle excitations in solids. The GW approximation (GWA) [1] is a well established approach for describing quasi-particle (QP) peaks in the one-particle spectral function. Beyond the GWA, the cumulant expansion approach (CEA), which is based on a quasi-boson model, gives a better description of the plasmon satellites [2,3,4] in many systems. However the traditionally used CEA, which is refereed to as the time-ordered cumulant (TOC), is designed for core level photoemission. Its performance for valence photoemission is less studied. In order to clarify the difference between different CEAs and their performance, in this talk I will show the most recent studies on the CEA including the TOC, and its generalized version that has been refereed to as the retarded cumulant (RC) [5], as well as further developments that go beyond these approximations. Two hole-plasmon coupling model Hamiltonians are chosen as benchmark systems and results for real materials are discussed.

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Poster Contributions

First principal calculations of optical and electrical properties of Sc, Ti and V doped SnO_2 used in photovoltaic applications

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The full-potential linearized augmented plane wave method (FP-LAPW) based on the density functional theory (DFT) and Boltzmann's Transport theory, are employed to investigate theoretically the electronic structure, optical and electrical properties of Sc, Ti and V doped rutile SnO_2. The FP-LAPW based on the new potential approximation known as the Tran–Blaha modified Becke–Johnson exchange potential approximation (mBJ). The calculated band structure and density of states (DOS) exhibit a band gap of pure SnO_2 (3.3 eV) closer to the experimental one. As well, our results indicate that the average transmittance in the 400 to 1000 nm wavelength region was 90%. The high transmittance and electrical conductivity indicate that hexagonal doped SnO_2 system is a potential as material for solar energy applications.

Non radiative degradation mechanism in FIrpic: blue phosphorescent OLED emitter

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The use of phosphorescent organic molecules in OLEDs offer the potential of using both the singlet and triplet excitons in realizing 100% internal quantum efficiency of electroluminescence. However, the injected charge carriers (electrons and holes) may become trapped, thus yielding to the accumulation of non-radiative recombination centers and luminescence quenchers at morphological and chemical defects. However, a microscopic understanding of the efficiency "roll off" of OLEDs is still lacking to date. Therefore the study of degradation pathways, ultimately leading to device aging and failure, is essential to meet the device lifetime and efficiency requirements [1]. *FIrpic* is one of the most used blue emitter used in OLEDs. Under high current density, there is an experimental hint that it degrades by loss of fluorine and/or the loss of picolinate ligand, but the mechanism is yet unclear [2,3]. In order to shed light on the dissociation pathways, we performed Car-Parrinello molecular dynamics with constrained orbital occupations to simulate the presence of an excitation (electron, or hole polaron and an electron-hole exciton pair), as if it were electrically injected into the device. We observed first the dissociation of the picolinate, which at a later stage can dissociate into CO_2 and $C_5H_4N^+$ fragments, leaving a four-fold coordinated Ir. Additionally, we determined the dissociation energies of the bonds involving the central Ir at the B3LYP level. In experiments, we built several FIrpic-based devices, and analyzed the various fragments found in the mass spectra of aged devices. Our results confirm the dissociation of the picolinate ligand is the most probable especially in presence of an electron-hole, but the substitution of the picolinate with a dfppy ligand greatly enhances the device lifetime.

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Quasiparticle Self-consistent GW and the Bethe Salpeter equation

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Determining the electronic structure of solids has become a vibrant field of research within the Physical sciences over the past century. One widely used method is that of Hohenberg, Kohn and Sham's density functional theory (DFT). Despite its success and wide use this formalism has many drawbacks; for example, in the study of systems excited beyond their ground state. Here we use a many-body perturbation theory (MBPT) approach: referred to as quasiparticle self-consistent GW (QSGW) [1]. This approach determines the 'best' unperturbed Hamiltonian (by an iterative procedure) to which the perturbation should be added; as opposed to the majority of MBPT calculations in the past that employed Hedin's GW approximation [2] using DFT (in particular the LDA) eigenfunctions and eigenvalues to generate the Green's function. This approach here - in theory - has the advantage of being independent of DFT. Optical absorption is a situation where we have a system of electrons in an excited state. The absorption of a photon creates an interacting electron-hole pair (an exciton), and to calculate the absorption spectra accurately one must go beyond the usual random phase approximation. The Bethe-Salpeter equation — containing the two-particle Greens function (a 4 point object) — is used to describe such processes. We introduce the Bethe-Salpeter equation, and discuss its implementation within a full-potential all-electron QSGW code: based on the linear muffin tin orbital approach [3]. Spectra for a few cases will be presented. The polarisation determined with the Bethe-Salpeter Equation can then be used to calculate many other properties of the system under investigation.

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Spin-state transition in unstrained & strained ultra-thin BiCoO$_3$ films

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Using first principles density functional theory (DFT) based calculations supplemented with the Hubbard U term (DFT+U), we theoretically study the structural, electronic and magnetic properties of ultra-thin films of a perovskite compound BiCoO$_3$, constructed along the [001] direction under ambient conditions. Our study shows that significant structural change occurs in thin-film geometry compared to bulk, which modifies the local oxygen coordination around the Co ion from a square pyramidal environment in the bulk phase to an octahedral environment in the thin-film structure. This changes the high-spin state of Co^{3+} in bulk to the low-spin state of Co^{3+} ions in the thin-film geometry. The influence of both tensile and compressive strain on the structural and electronic properties of the thin-film is studied. Our study shows a layer selective transition of the Co^{3+} spin state when subjected to tensile strain, which is found to be driven by the change in the Bi environment. Our theoretical study should motivate the experimental investigation of the thin film of BiCoO$_3$.

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Two step phase transition in SnSe and the origins of its high powerfactor from first principles

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The interest in improving the thermoelectric response of bulk materials has received a boost after it has been recognized that layered materials, in particular SnSe shows a very large thermoelectric figure of merit. This result has received a large attention while it is now possible to conceive other similar materials or experimental methods to improve this value. Before we can now think in engineering this material it is important we understand the basic mechanism that explains this unusual behavior, where very low thermal conductivity and high thermopower result form a delicate balance between crystal and electronic structure. In this paper, we present a complete temperature evolution of the thermoelectric properties as the material undergoes a soft crystal transformation and its consequences on other properties within SnSe by means of first principles calculations. Our results are able to explain the full range of considered experimental temperatures. The huge figure of merit found experimentally is due to a combination of high electrical conductivity, sustained Seebeck coefficient, and low thermal conductivity. We show that two interrelated effects are determinant, the formation of defects and the structural phase transition from Pnma to Cmcm. The different defect energetics in the two phases gives rise to an order of magnitude increase in the carrier concentration, and therefore also the conductivity, counteracting the increase of electron scattering with temperature. The defects and carriers appear progressively as the Pnma phase also regularizes its structure towards the Cmcm high-temperature phase. We show that the stability of the high-temperature phase is ensured by strong anharmonic effects. The corresponding Seebeck coefficient is slightly lower in the Cmcm phase, but this is more than offset by the increase in conductivity. We finally analyze the microscopic mechanisms behind the phase transition, which combines elastic and vibrational distortions.

Vibrationally pumped spectra of the ET-F$_2$TCNQ crystal

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Strongly correlated electronic systems are characterised by large electron-electron repulsive interactions that cannot be treated at a mean-field level or in a perturbative way. The phase diagram of such systems is often complicated, showing very different phases for even slight changes of external parameters, like applied electric/magnetic field, pressure, etc. More recently, ultrashort light pulses were used in order to create out-of-equilibrium many-body configurations and to follow in real time the dynamics of nuclear and electronic degrees of freedom. Recently, Kaiser et al.[1] and Singla et al.[2] realized ultrafast pump-probe experiments on the charge-transfer segregated-stack crystal ET-F$_2$TCNQ, a prototypical 1D Mott insulator. More precisely, they selectively excited a non-totally symmetric (non-ts) ET molecular vibration with a mid-infrared ultrashort light pulse ($\sim$130 fs) and induced charge-transfer along the stack of still vibrating ET units. As a result, they observed a transient change in the reflectivity signal (70 cm^{-1} red-shift of the $\sim$5600 cm^{-1} CT band, as well as three new bands, at 4200 cm^{-1}, $\sim$3000 cm^{-1}, $\sim$2000 cm^{-1}) and ascribed it to a coherent modulation of the Hubbard U induced by the ET driven mode. We theoretically describe the experiments reported in [1] and [2]. Focusing on just two ET molecules, we start from an Hubbard dimer model and, introducing in a non-adiabatic way the coupling to a non-ts molecular vibration, we propose three different model Hamiltonians: **model A**, where vibrational frequency changes with the charge residing in the ET frontier molecular orbital; **model B**, where non-ts molecular vibration modulates the nearest-neighbour electrostatic interaction, V, and **model C**, where it modulates the on-site electrostatic interaction, U. Using quantum chemistry methods (DFT), we estimate electron-vibration coupling constants for the three models. Exact (numerical) diagonalization of the three Hamiltonians gives fully non-adiabatic eigenvectors, used to calculate optical spectra. Neither model A, nor model B describes the transient changes experimentally observed, while model C, in agreement with [1] and [2], captures the 70 cm^{-1} red-shift of the CT band. Indeed, none of the three models explain the three additional bands experimentally seen at lower frequencies, thus suggesting their possible different origin.

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Photoemission Spectra from Reduced Density Matrices: the Band Gap in Strongly Correlated Systems

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We present a method for the calculation of photoemission spectra in terms of reduced density matrices. We start from the spectral representation of the one-body Green's function G, whose imaginary part is related to photoemission spectra, and we introduce a frequency-dependent effective energy that accounts for all the poles of G. Simple approximations to this effective energy give accurate spectra in model systems in the weak as well as strong correlation regime. In real systems reduced density matrices can be obtained from reduced density-matrix functional theory. Here we use this approach to calculate the photoemission spectrum of bulk NiO: our method yields a qualitatively correct picture both in the antiferromagnetic and paramagnetic phases, contrary to mean-field methods, in which the paramagnet is a metal.

Magnetic structure of the noncentrosymmetric heavy-fermion superconductor CePt$_3$Si

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The tetragonal heavy-fermion compound CePt$_3$Si has attracted strong attention from both experimentalists and theoreticians in recent years because it shows unconventional superconductivity despite its noncentrosymmetric crystal structure. The lack of inversion symmetry leads to an antisymmetric spin-orbit coupling, which mixes spin-singlet and spin-triplet Cooper-pairing channels. This so-called Rashba-type spin-orbit coupling also leads to an anomalous dynamic spin susceptibility as revealed by polarized inelastic neutron scattering [1]. The superconducting transition occurs at $T_c = 0.75$ K, well inside the magnetically ordered state that sets in at $T_N = 2.2$ K. The magnetic structure is characterized by a propagation vector k=(0,0,1/2), and is supposed to consist of sheets of ferromagnetically ordered moments aligned in the a-b plane, the sheets being stacked antiferromagnetically along the c axis. However, the direction of the moments in the a-b plane is fully unknown. Also, the magnitude of the ordered moment, which is strongly reduced in zero magnetic field, has been reported to increase substantially with increasing magnetic field [2], which is a quite unusual and puzzling behavior. We have redetermined the magnetic structure using elastic polarized neutron scattering with field-projected (longitudinal) XYZ polarization analysis on the IN20 triple-axis spectrometer, using a set-up with Heusler monochromator and analyzer and a Helmholtz coil at the sample position. Care was taken to minimize contributions of unpolarized higher-order neutrons from the monochromator. We find that the magnetic structure is different from what has been assumed hitherto. This has strong implications for the magnetic phase transition and the low-temperature structure of the system, and could provide a key explanation to the unusual magnetic field dependence of the ordered moment.

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First-principles study of Resonant Raman Scattering including Exciton-Phonon Interaction

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A resonance phenomenon appears in the Raman response when the exciting light has frequency close to electronic transitions. Unlike for molecules and for graphene, the theoretical prediction of such frequency-dependent Raman response of crystalline systems has remained a challenge. Indeed, many Raman intensity first-principle calculations are nowadays done at vanishing light frequency, using static Density-Functional Perturbation Theory, thus neglecting the frequency dependence and excitonic effects. During this presentation, I will describe the finite-difference method we propose to compute frequency-dependent Raman intensities. Recently, we used this methodology for the computation of the first-order frequency-dependent Raman intensity [1], with excitonic effects described by the Bethe-Salpeter equation. We found these to be crucial for the accurate description of the experimental enhancement for laser photon energies around the gap. This approach can be generalized to the more complex second-order Raman intensity, with phonon losses coming from the entire Brillouin zone. Interestingly, even without excitonic effects, one is able to capture the main relative changes in the frequency-dependent Raman spectrum at fixed laser frequencies. However, excitonic effects might affect significantly the intensity of specific modes and also lead to a global tenfold increase of absolute intensities.

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Local Field Effects for surfaces or thin films optical properties

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Time Dependent Density Functional Theory in reciprocal space is a tool of choice for obtaining optical properties of periodic crystals. For surfaces or thin films, the periodicity is lost in the perpendicular direction. However, the same framework can be used to calculate the susceptibility, thanks to a supercell with alternate slabs of matter and vacuum. A measurable quantity related to the susceptibility is the absorption spectrum. We show that the supercell method gives the correct absorption spectra for the in-plane directions, but fails for the perpendicular one, when the response to the external macroscopic potential accounts for inhomogeneities at the atomic scale (LFE). In this case, the method is equivalent to an effective medium theory for a slab of material and vacuum, the absorption spectrum is shifted towards high energy and converges towards the Electron Energy Loss spectrum for large vaccum. We show that the problem comes from the use of a periodic system to describe a non-periodic one when solving the Dyson equation relating the susceptibility and the polarisability. We propose a new scheme called "selected G"[1], which allows the inclusion of LFE in the absorption spectrum perpendicular to the isolated thin film. We illutrate this work on a silicon slab.

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The Flavours of the Self-Interaction Correction

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The self-interaction correction is a method to improve upon the local-density approximation by introducing and additional term to the Hamiltonian that removes those contributions to the Hartree and exchange-correlation potentials experienced by each electron due to its own density. This additional term means that each electron experiences a different total potential and breaks the invariance of the Hamiltonian under unitary transformations of the electronic wave functions. In particular, the method formally distinguishes between localised and Bloch states and, by considering the total energy, it is able to predict the localisation-delocalisation transitions due to, e.g, chemical environment or pressure. Because of the ability to treat localisation, the self-interaction correction approach is a very valuable method to examine d- and f-electron systems where the varying number of localised states plays a crucial role. We discuss the benefits and drawbacks of the method and its implementation in a Wannier basis as well as approximate local correction methods.

Core-Level Spectra in the Dynamical Mean-Field Theory

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The combination of the local-density approximation with the dynamical mean-field theory (LDA+DMFT) is a capable method for first-principles investigation of materials with correlated electrons. Although it is primarily devised for the valence-band electronic structure, LDA+DMFT provides a means to calculate also core-level spectra at the level of the so-called multiplet ligand-field theory, with little to no empirical input. We employ this method to analyze differences between core-level spectra of selected actinide and lanthanide oxides, and to investigate the electronic structure od lanthanide adatoms on metallic surfaces, such as holmium on Pt(111).

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Self-consistent combination of the GW-approximation and Dynamical Mean-Field Theory: Example SrVO$_3$

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We present the first fully self-consistent combination of the *GW*-approximation and dynamical mean-field theory (DMFT) applied to SrVO$_3$, considered a prototype of a strongly correlated material. The experimental spectra of SrVO$_3$ exhibits a pronounced quasi-particle peak in between two satellite features, which have previously been interpreted as upper and lower Hubbard bands. Within a consistent treatment of both local correlations within DMFT and non-local correlations within the *GW*-approximation we show that this interpretation is not correct. While the correct three-peak structure is retained the effective impurity interaction is reduced by the strong non-local screening and the features previously identified as Hubbard bands are re-interpreted as being plasmon satellites. Our work highlights the important role of non-local screening processes and correlations and shows that a proper treatment of these effects can drastically change the physical interpretation of the spectra. This is expected to be the case for a wide range of materials. e-mail corresponding author : dzovan90@gmail.com

A dynamic exchange correlation kernel derived from recent results for the homogeneous electron gas

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Time-Dependent Density Functional Theory (TDDFT) is a method of choice to calculate the dynamic structure factor of a wide range of materials. Even in the simplest Adiabatic Local Density Approximation (ALDA), plasmon spectra are generally well described. However, several shortcomings remain. In particular, the onset energy of the spectrum is underestimated [1], and dynamical effects such as lifetime damping and double plasmon excitations are absent [2]. In this work we investigate recent results for the dynamic response of the homogeneous electron gas (HEG)[3] to extract an exchange correlation kernel for TDDFT. In order to get an estimate of the validity of such an approach we compare our results for the dynamic exchange correlation kernel $f_{xc}(q,\omega)$ for the homogeneous electron gas with different kernels and known exact properties, and we test results on simple metals.

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DFT and beyond with the Electronic Structure Library

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The accelerating pace of technology, with its new architectures, new models, new processes, new tools, as well as with its data-oriented priorities, is creating higher and higher challenges for scientists on a daily basis, requiring collaborations to include more and more disciplines to be successful. By providing high-quality DFT codes and interoperability standards to the electronic-structure community, and due to its intrinsic friendly attitude towards multidisciplinary endeavors, the ETSF has layed a rock-solid basis for other initiatives, such as the Electronic Structure Library (ESL), which aim at meeting these challenges by creating new alliances.

The ESL is a long-term project which can be considered, at the same time, as:

- a digital library, materialized by a wiki, where researchers developing new theories and software find useful information and tools to stop reinventing the wheel and accelerate the realization of their projects;

- a repository of free (libre) software of general interest for the electronic-structure community, permanently open to contributions;

- a software development infrastructure and meeting space for electronic-structure scientists.

Its ultimate goal is to provide researchers with stable, optimized, well-tested, and well-documented, low-level software components for the development of new theories, in a way that lets them focus on what they are best at: science. To achieve it, the ESL contributors have devised specific collaborative strategies, processes and tools to make constant progress towards offering Lego®-like components to build electronic-structure software. They meet regularly thanks to CECAM-sponsored workshops.

See http://esl.cecam.org/ for more information.

Ground- and Excited-State Properties of Orthorhombic MAPbI$_3$

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Hybrid organic-inorganic halide perovskites are one of the most promising candidates for the next generation of photovoltaic devices with high power-conversion efficiencies. Despite the amazing progress in device fabrication, many of the fundamental properties of these materials are not yet understood. The flexibility in composition of hybrid perovskites permits to tune physical properties like band gap, dielectric constant, or optical absorption which renders them interesting also from a fundamental point of view and for applications beyond photovoltaics. The most intensively studied compound, methylammonium lead iodide (MAPbI$_3$), condenses in a low-temperature orthorhombic phase which undergoes a phase transition to a tetragonal structure at 162.2 K and transforms into a cubic high-temperature phase above 327.4 K. These phase transitions go along with a change in the optical properties. Here, we focus on the orthorhombic phase of MAPbI$_3$. We have studied the ground-state atomic structure, and in particular the orientation of the MA$^+$ ion within the inorganic cage, within density-functional theory. We investigate the one-particle excitation properties (band gap, photoemission spectrum) within the GW approximation of many-body perturbation theory. Moreover, we calculate optical and loss spectra using time-dependent density-functional theory and solving the Bethe-Salpeter equation.

An efficient calculation method for van der Waals coefficients based on Krylov subspace technique

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First-order perturbation calculations are frequently appeared in quantum dynamics as kinds of response function, e.g. optical absorption spectra, microscopic dielectric function within many-body perturbation theory, and van der Waals (vdW) coefficient calculation. In order to obtain both real and imaginary components of them with spectral representation, large amount of eigenfunction and corresponding eigenvalue are needed in order to achieve convergence, leading to formidable calculation cost sometime. A way to avoid the huge spectral information is employing a set of linear equations varying different frequencies. We apply this strategy to evaluate vdW coefficients as an example of the response functions. General response function is cast as $\langle a|AG(\omega)B|a\rangle$, where a is a state, A, B are operators, and $G(\omega)$ is a Green's function with frequency ω. By solving a linear equation $(\omega I - H)|x(\omega)\rangle = B|a\rangle$, the response function is obtained as $\langle a|x(\omega)\rangle$. The linear equation is categorized as shifted linear equation in applied mathematics and able to be solved by use of shifted Krylov solvers. We have developed a more efficient approach, in the sense of numerical calculation cost and required memory, to obtain just response function avoiding explicit solution of linear equations, named as reduced shifted subspace solver(RSKS) [1] and applied it to Green's function in Bogoliubov de Gennes equation. We will present how RSKS works well for the calculation of vdW coefficient and actual performance of calculation point of view.

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A Space-Time Study of the Electron-Electron Interaction in High-T_c Parent Compound La$_2$CuO$_4$: In Search of an Attractive Effective Interaction

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The superconductivity under doping in the famous cuprate compounds is believed to originate in the CuO$_2$ planes. The mediator of pairing is generally accepted to be derived from electronic degrees of freedom. While many mechanisms, such as spin fluctuations, have been proposed throughout the years, little research has been carried out on the role of retarded attraction due to electronic overscreening.

In this study, the dynamically screened interaction $W(\mathbf{r}, \mathbf{r}'; t)$ is studied in the CuO$_2$ planes of the parent compound La$_2$CuO$_4$. To this end, a repulsive test charge, representing an electron, is introduced at various $\mathbf{r}'$ in the CuO$_2$ plane, and $W(\mathbf{r}, \mathbf{r}'; t)$ is calculated as a function of $\mathbf{r}$ and t. The aim is to explore the possibility of the existence of an attractive effective interaction between electrons. The static screened interaction $W(\mathbf{r}, \mathbf{r}'; \omega = 0)$, which is the time average of $W(\mathbf{r}, \mathbf{r}; t)$ is also studied. In addition, the effective interactions $U_1(\mathbf{r}, \mathbf{r}'; t)$ and $U_3(\mathbf{r}, \mathbf{r}'; t)$, corresponding to the well-known one- and three-band models, are investigated using the constrained random-phase approximation (cRPA). Substantial regions of the CuO$_2$ plane do indeed exhibit an attractive effective interaction U_1/U_3. On the other hand, the extent of such regions is significantly smaller in SrVO$_3$, a *non-superconducting* metal.

The present work suggests that future studies of electronic overscreening as a possible pairing mechanism is worth consideration. The same *ab initio* parameters as obtained and utilized in this work can be used to construct a Hubbard-Holstein model, from which the gap function can be calculated by solving the Eliashberg equations.

A Strong Coupling Approach to Transition Metal Dichalcogenides

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Based on a strong-coupling approach [1], we analyze the recent experiments on layered transition metal dichalcogenides (TMD) that contradict traditional views of the charge density wave (CDW) arising out of nested bands [2]. The discovery of superconductivity in 1T-TiSe2 and other TMDs [3] has added a new dimension to the problem. A high-temperature bad metallic, non-Fermi liquid state becoming more coherent in the broken symmetry state is fundamentally at odds with a mean-field picture [2]. The very high transition temperature obtained from electron-phonon mechanism [4] also shows its inadequacy. A strong-coupling view of the CDW arising as a Bose condensation of preformed excitons emerges as a possible, albeit rarely discussed alternative. Revisiting some of these systems [1], we explain a host of normal state data that appear to be fairly generic. A local density approximation plus multi-orbital dynamical mean field theory calculation shows that the present approach makes good contact with extant normal state data. The incoherent normal state arises out of the coupling between putative qusiparticles and soft excitonic fluctuations. It is also argued that the broken symmetry states at low temperature are instabilities of such a strongly correlated excitonic liquid.

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Excitons in Graphene/hBN nanostructures

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Two dimensional semiconductors have recently attracted a tremendous amount of attention, with mono-layers of hexagonal boron nitride (hBN) representing a prime example. Reduced screening and confinement effects in this materials leads to an optical response completely dominated by strongly bound excitons. Graphene, on the other hand, is a semi-metal in which excitonic effects are much less pronounced. This fundamentally different optical behavior spurs the question as to the importance and underlying physics of correlated electron-hole pairs in hybrid graphene/hBN monolayer materials. In this talk, we consider the optical response of graphene/hBN in-plane (lateral) super-lattices, which are essentially adjacent nano-ribbons composed of alternating graphene and hBN. We model the electronic structure, consider effects of correlated electron/hole pairs (i.e. excitons) in a Bethe-Salpeter formulation, and discuss also the possibility for molecular electric field induced second-harmonic generation in the graphene domains due to the asymmetry of B and N terminated graphene edges.

Building approximations to capture excitonic effects of correlated electrons

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The state-of-the-art *ab initio* method to describe electronic excitations in solids is the solution of the Bethe-Salpeter equation (BSE) based on a Kohn-Sham electronic structure with GW quasiparticle corrections for the energy eigenvalues. For many solids, ranging from sp semiconductors to correlated insulators with open d shells, strong cancellation effects between the GW quasiparticle corrections and the electron-hole attraction (BSE) are found. To reveal correlation effects beyond GW we propose a reformulation of the original set of five Hedin's equations [1]. The improved description of correlation and the understanding of the cancellation mechanisms may guide the search for new exchange-correlation kernels that can capture also excitonic effects [2].

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Effective Approaches for Electron Spectroscopy

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Effective approaches using auxiliary systems constitute an attractive and pragmatic strategy to deal with the direct calculation of specific quantities of interest, that are otherwise obtained from computationally expensive many-body wavefunctions or Green's functions. A prominent example is density functional theory, in which the Kohn-Sham system [1] is built to yield the electronic density in an efficient way. Analogously, in order to describe the results of photoemission experiments, another auxiliary system [2] can be set up: it reproduces the exact spectral function, which is usually evaluated from a complex non-local self-energy, with a real, local and frequency-dependent potential. I have applied this method to the one-electron symmetric Hubbard dimer, deriving the local and frequency dependent effective potential, that turns out to be dense of physical meaning. In a second step, generalizing the standard DFT LDA to a dynamic approach, I have used the exact symmetric result to study the spectral function of the corresponding asymmetric system, exploring several approximations to the effective potential. Finally, I have considered the electron gas in different screened Hartree Fock approximations, in order to design a good model system potential to be used for describing real system spectral functions.

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Huge anisotropic exchange and exotic magnetism in honeycomb and pyrochlore iridates

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Large anisotropic exchange couplings in 5d oxide compounds open the door to new types of magnetic ground states and excitations, inconceivable a decade ago. In honeycomb Na_2IrO_3, for example, the intersite spin-coupling anisotropy shows up in the form of bond-dependent Kitaev interaction terms; this symmetric anisotropic exchange (K) defines in Na_2IrO_3 the leading magnetic interaction term. For nearest-neighbor IrO_6 octahedra in Sr_2IrO_4, on the other hand, the key anisotropy is the antisymmetric contribution (D); it reaches impressively large values of about 15 meV, orders of magnitude larger than in, e.g., the isostructural '214' cuprates. We discuss the promise for exciting Kitaev-Heisenberg physics in 5d (Ir) and 4d (Rh, Ru) oxide and halide honeycomb systems. In particular, the dependence of the Kitaev K and Heisenberg J couplings on bond angles is analyzed, by using quantum chemistry calculations [1,2]. We also explore computationally ways of achieving large D/J ratios in pyrochlore iridates and predict a regime in which D>5 meV and J–¿0. Such iridates provide thus ideal playgrounds to investigate for instance skyrmionic states of the type anticipated by the Uppsala group [3].

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Maps

TRAIN
TO / FROM
CPH
AIPORT

P-hus

Central
station

Allhelgonakyrkan

BUS
Pickup
Point

Main locations:

1. Eden Venue
   (main conference)
2. Palaestra Venue
   (Friday location)
3. Tegnérs
   matsalar (food)
   (lunch Tue 20th &
   Fri 23rd)
4. Kulturen (food)
   (lunch Thu 22nd)
5. Stäket (food)
   (lunch Wed 21st)

Domkyrkan
(Cathedral)

Hotel
Concordia H

BUS
Pickup
Point

Hotel
Nordic H

BUS
Pickup
Point

Stadsbussar
(City buses)

Mårtenstorget

Länsbussar
(County buses)

Stortorget

P-hus

Brita Holm-
ströms gata
Fredsgatan
Karl XI gatan
Sankt Laurentiigatan
Bredgatan
Allhelgona Kyrkogat
Helgonavägen
Finngatan
Sölvegatan
Biskopsgatan
Clemenstorget
Sankt Petri Kyrkogat
Sandgatan
Paradisgatan
Tomegap
Byaregatan
Adelgatan
Knut den stores torg
Lilla Gråbrödersg
Nunnegatan
Gråbrödersgatan
Stora
Kyrkogatan
StoraAlgatan
Klostergatan
Bantorget
Lilla
Tegnérsplatsen
Krafts-
torg
Magle Stora Kyrkogata
Lilla Algatan
Agardhsgatan
Östra Vallgatan
Trollebergsvägen
Fiskaregatan
Stålbrogatan
Västergatan
Nygatan
Åtta kant sund
Skomakaregatan
Killiansgatan
Magle Lilla Kyrkogata
Laboratoriegatan
Östra Mårtensgatan
Västra Mårtensgatan
Drottensgatan
Södergatan
Stora
Bankgatan
Lilla Tvärgatan
Råbygatan
Skolgatan
Vallgatan

Restaurants & Pubs (with food)

1. Grand hotel ($$)   8. Bishop's Arms Pub
2. Italia   9. Klostergatans vin
3. Gloria's   & delikatess
4. John Bull Pub   11. Stortorget
5. GattoStretto   12. Pintxos
6. RoseGarden   13. Inferno
7. M.E.A.T.   14. Ishiri