Report on the 2008 "Computational Physics and Materials Science" Mini-Workshop in Bonn, Germany

**International Workshop on
Computational Physics and Materials Science:
"Progress in Computational Electronic Structure Theory"**

10-12 January 2008
Gustav-Stresemann-Institut, Bonn, Germany

Organizers:

Erik Koch and Eva Pavarini
Institut für Festkörperforschung, FZ-Jülich

Web page:
http://www.i2cam.org/conference/cpest/

The workshop was part of the series of International Workshops on Computational Physics and Materials Science, which started in Oxford (1983) and Braunschweig (1984), and is continued biennially in Trieste (1987, ..., 2007), with mini-workshops in the intervening years (2004: Paris, 2006: Cambridge). The 2008 edition was organized with the help of the Forschungszentrum Jülich at the Gustav-Stresemann-Institut (GSI) in Bonn, Germany.

As the previous workshops, this year's meeting served to survey the state-of-the-art of computational methods for the calculation of the electronic structure of real materials. A special focus was recent progress in the understanding of correlated systems beyond simple model systems. The aim was to bring together practitioners from different parts of the electronic structure community and to enable the exchange of ideas between the fields ranging from method development to applications.

The workshop was attended by 43 participants staying at the GSI plus 8 students commuting from Bonn University and Jülich. Thanks to financial support from the the Forschungszentrum Jülich, the European Science

Foundation (ESF) through psi-k, and the Institute for Complex Adaptive Matter (ICAM), we could cover the local costs of all participants. In addition, with the help of ICAM Junior Travel Awards, we were able to cover the travel expenses of three young participants, a PhD student from China as well as two postdocs, one from Bangladesh and one from the United States.

The program consisted of 20 invited talks (50 minutes with ample time for discussion) that presented recent advances in the field. The chairs played the key role of stimulating and directing the animated discussions on the work and its perspective in the field. All presentations are available at http://i2cam.org/conference/cpest/. The program also involved a lively poster session with 13 contributions. The GSI, with all facilities (lecture room, accommodation, and cafeteria) located in the same building, proved to stimulate discussions to extend well beyond the regular workshop program.

The talks provided a rich sampling of recent developments in electronic structure theory with a certain focus on new methods for systems with electron correlations.

The first session was devoted to quantum Monte Carlo, where in the context of traditional diffusion Monte Carlo J. Toulouse presented a new approach to wave-function optimization while M. Casula discussed how to deal with non-local pseudopotentials. New developments in determinant-based methods were S. Zhang's auxiliary-field Monte Carlo for ground- and even excited states as well as the continuous-time QMC approach developed by A. Rubtsov, which is establishing itself as the solver of choice for dynamical mean-field theory.

The afternoon was devoted to large systems and surfaces: L. Genovese demonstrated how a wavelet basis can be used for efficient bigDFT calculations. Applications to processes at surfaces were presented by M. Bernasconi, discussing the dynamics of silyl radicals on silicon, D. Alfè, who presented a technique for computing thermal desorption rates and gave an outlook on how to include nuclear quantum effects. Finally J. Behler demonstrated how to treat non-adiabatic effects using constrained DFT.

On friday morning the focus was on excited states. The strength of combining methods for the calculation of optical spectra was demonstrated by O. Pulci for the combination of many-body perturbation theory and molecular dynamics and by R. Gebauer combining time-dependent DFT with Lanczos. Going to finite temperatures, A. Marini showed how to calculate excitons a experimental temperatures, while M. Verstraete presented an extension of the space-time formulation of GW to finite-T, giving applications to metallic systems.

In the afternoon new methods for strongly correlated electrons were discussed. F. Aryasetiawan explained how to determine ab-initio parameters for model Hamiltonians and gave exciting examples. I. Souza demonstrated the amazing accuracy of Wannier interpolation techniques. Focusing on many-body physics, S. Savrasov discussed the locality of the self-energy in real space, which is so central to methods based on dynamical mean-field theory, while M. Potthoff gave an introduction to his new self-energy functionals.

The final session on Saturday was devoted to applications to strongly correlated materials. After a comprehensive overview of the current state-of-the art of the field by A. Lichtenstein, K. Haule discussed how heavy Fermion systems can be realistically modeled. R. Valenti discussed the intricacies of orbital ordering in a frustrated spinel. Going beyond bulk systems, R. Pentcheva presented the interesting physics that makes the interface between two insulators metallic.

Program

Thursday, 10 January 2008

8:45	Welcome
chair:	R. Needs
9:00	S. Zhang: *Recent progress in auxiliary-field electronic-structure methods*
9:50	J. Toulouse: *Optimization of quantum Monte Carlo wave functions by energy minimization*
10:40	coffee
11:00	M. Casula: *Diffusion Monte Carlo methods with non-local potentials*
11:50	A. Rubtsov: *Continuous time QMC methods: Applications for DMFT and beyond*
12:40	lunch
chair:	X. Gonze
14:30	L. Genovese: *Daubechies wavelets as a basis set for density functional pseudopotential calculations: the BigDFT project*
15:20	M. Bernasconi: *Adsorption, diffusion and decomposition of silyl radicals at clean and hydrogenated Si(100) surfaces by ab-initio simulations*
16:10	coffee
16:40	J. Behler: *Non-adiabatic effects in the oxygen dissociation at the Al(111) surface*
17:30	D. Alfè: *Absolute rate of thermal desorption form first-principles simulations*
20:00	Poster session

Friday, 11 January 2008

chair: X. Gong

9:00   A. Marini: *Ab-initio finite temperature excitons*

9:50   O. Pulci: *Optical spectrum of water: many-body perturbation theory meets molecular dynamics*

10:40   coffee

11:00   R. Gebauer: *A Lanczos-based recursion scheme for the direct calculation of optical spcetra in TD-DFT*

11:50   M. Verstraete: *The GW space-time formalism at finite temperature for metallic systems*

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14:30   S. Savrasov: *Are self-energies local? Insights from LDA+DMFT and GW+DMFT*

15:20   M. Potthoff: *Lanczos-based cluster methods for strongly correlated electron systems*

16:10   coffee

16:40   F. Aryasetiawan: *Calculating the Hubbard U from first principles: Constrained RPA*

17:30   I. Souza: *Wannier interpolation and its application to the calculation of anomalous Hall conductivity*

20:00   Conference dinner

Saturday, 12 January 2008

chair: M. Gillan

9:00   A. Lichtenstein: *Spectral density functionals: LDA+DMFT*

9:50   K. Haule: *Modeling the localized-to-itinerant electronic transition in the heavy Fermion system $CeIrIn_5$*

10:40   coffee

11:00   R. Pentcheva: *Compensation mechanisms and functionality of perovskite interfaces*

11:50   R. Valenti: *Orbital order in the frustrated spinel ZnV_2O_4*

Participants

Alfè, Dario — University College London, UK

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International Workshop on Computational Physics and Materials Science

Progress in Computational Electronic Structure Theory

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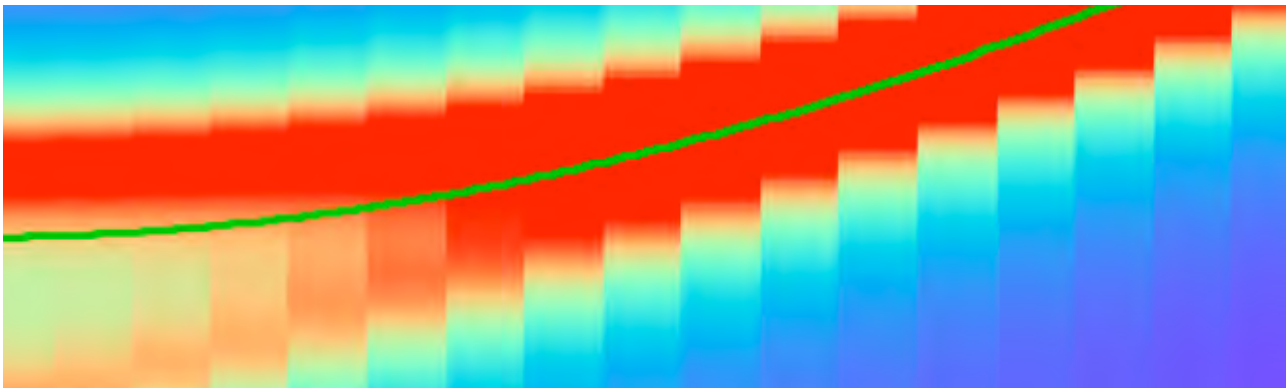
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Abstracts

Absolute rate of thermal desorption from first-principles simulations

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We present a technique for computing by first-principles simulation the absolute desorption rate   of adsorbate molecules from a surface for any coverage and temperature. The technique is valid when the thermal equilibration rate on the surface is faster than   , and is based on an exact expression for   in terms of the difference of non-configurational chemical potentials of gas-phase and adsorbed molecules. This difference is expressed in terms of a potential of mean force (PMF), which is computed by constrained first-principles molecular dynamics. The technique is applied to H_2O on the MgO(001) surface at low coverage, using the generalised gradient approximation (GGA) for exchange-correlation energy. Nuclear quantum effects have been studied with the path-integral technique. Comparisons with experimental TPD data allow an assessment of the accuracy of GGA for the adsorption of H_2O on MgO(001). Preliminary quantum Monte Carlo results will also be presented.

Calculating the Hubbard *U* from first principles: Constrained RPA

Ferdi Aryasetiawan

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Recent development in materials science has revealed rich properties of materials containing 3*d* and 4*f* elements, notably when the 3*d* or 4*f* shells are partially filled, leading to strong on-site correlations. The LDA often fails qualitatively in treating these systems and the GW approximation, while able to partly improve the LDA, is not expected to cure most of the problems. However, due to the large number of degrees of freedom, it is very hard to improve upon the GW approximation using conventional diagrammatic methods in order to be able to treat systems with strong on-site correlations. On the other hand, model approaches have been rather successful in treating strongly correlated materials, albeit not from first-principles.

It is therefore highly desirable to be able to construct reliable model Hamiltonians where the input parameters are computed from first-principles, thus avoiding adjustable parameters which may lead to misleading results. Here we propose a constrained random-phase approximation (cRPA) scheme [1] that allows for a systematic down-folding of high energy screening channels resulting in a low-energy model Hamiltonian with a screened Coulomb interaction or the Hubbard *U* corresponding to an effective interaction among electrons living in an isolated and partially filled narrow 3*d* or 4*f* bands across the Fermi level. The model Hamiltonian can then be solved by sophisticated approaches such as the dynamical mean-field theory (DMFT) scheme. We have applied the cRPA method to the 3*d* transition metal series and to a couple of 4*f* systems (Ce, Gd) as well as a perovskite, $SrVO_3$. Comparison with the constrained LDA method will also be discussed [2].

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Non-adiabatic effects in the oxygen dissociation at the Al(111) surface

Jörg Behler

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The interaction of oxygen molecules with metal surfaces plays an important role in many technologically relevant processes like heterogeneous catalysis and corrosion. In recent years numerous experiments have shown that the oxygen dissociation at a series of metal surfaces is incompatible with an adiabatic description of the adsorption event.

A most basic and puzzling enigma has been in particular the dissociative adsorption of oxygen molecules at the Al(111) surface [1-4]. Using this system as an illustrative example we show that the experimentally well-established low sticking probability [1] of thermal oxygen molecules, which is in contradiction with state-of-the-art density functional theory (DFT) due to the absence of energy barriers on the calculated potential-energy surface (PES), is caused by spin-selection rules [5], which constrain the molecular motion to the initial spin-triplet PES of the free molecule. Employing a new locally-constrained DFT technique [6] we are able to demonstrate that this spin-triplet PES shows indeed energy barriers, which give rise to a low sticking probability in qualitative agreement with experiment. The obtained results are critically discussed with respect to inaccuracies in present-day exchange-correlation functionals. Some perspectives on the effect of electronic transitions from this triplet PES to the final singlet PES of the adsorbed atoms and on the dissociation mechanism [3,4] are given.

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[4] M. Schmid, G. Leonardelli, R. Tscheließnig, A. Biedermann, and P. Varga, Surf. Sci. **478**, L355 (2001)

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Adsorption, diffusion and decomposition of silyl radicals at clean and hydrogenated Si(100) surfaces by ab-initio simulations

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Plasma-enhanced chemical vapor deposition (PECVD) from silane is a widespread technique employed to grow thin films of amorphous silicon. High growth rates are made possible by the deposition of reactive radicals produced in the plasma (mostly SiH_3), as opposed to conventional CVD where the less reactive silane is directly adsorbed at the growing surface [1]. By suitably controlling the energy of the ions while keeping a high density of reactants, a related technique, called low-energy plasma-enhanced chemical vapor deposition (LEPECVD) [2] has introduced the possibility to obtain device-quality epitaxial films of crystalline silicon or silicon-germanium alloys, at temperatures much lower (600 C) than those necessary for conventional, thermal chemical vapor deposition (800 C). In spite of extensive investigation many atomistic details of the growth process by PECVD are still unclear.

In the long term perspective of modeling the PECVD growth of crystalline silicon, we have performed ab-initio simulations of adsorption, diffusion and decomposition of SiH_3 radical at the clean and hydrogenated Si(100) surface [3]. Ab-initio metadynamics technique has been used in the search of unbiased diffusion and decomposition pathways [4]. Transition state energies between different minima visited during metadynamics trajectories have been further refined by the Nudged Elastic Band (NEB) method. Competitive mechanisms for diffusion and desorption have been investigated by Kinetic Monte Carlo simulations based on ab-initio reactio rates. In particular, the role of atomic hydrogen present in the plasma in promoting SiH_3 diffusion and its epitaxial incorporation into the growing surface has been elucidated [5].

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Diffusion Monte Carlo methods with non-local potentials

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We show how to include non-local potentials in the diffusion Monte Carlo framework in a variational way, substantially improving both the accuracy and the computational stability upon previous non-variational diffusion Monte Carlo approaches. We will review and compare two methods, the lattice regularized diffusion Monte Carlo [1] and the non-local diffusion Monte Carlo [2], which are variational even in the presence of non-local pseudopotentials. These methods can open the route for even more reliable and accurate electronic structure calculations of the ground state by means of quantum Monte Carlo. We will present some recent applications.

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[2] M. Casula, Phys. Rev. B **74**, 161102(R) (2006)

A Lanczos-based recursion scheme for the direct calculation of optical spectra in TD-DFT

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In the most common approaches to time-dependent density functional theory, a system's excitation energies are computed as the eigenvalues of a large response operator. This requires the explicit diagonalization of the response operator in the energy range of interest. This is often a computationally very demanding task, and quickly becomes impossible if the system is very big, or if the energy range and basis set are very large. As an alternative to this approach, it is possible to avoid the diagonalization of the response operator completely, and to use a Lanczos-based recursion scheme for the direct calculation of optical spectra. This scheme allows one to quickly calculate the spectra even in large systems with huge (plane-wave) basis sets. In this presentation we will introduce the basic ideas behind this algorithm and show applications to systems of biological and technological interest.

Daubechies wavelets as a basis set for density functional pseudopotential calculations: the BigDFT project

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The EU-NEST BigDFT project has developed an ab-initio pseudopotential DFT code based on Daubechies wavelets. They are an orthonormal compact-support multiresolution basis, and form one of the few examples of systematic real space basis sets. For these reasons they provide good efficiency in expanding localized information. An ab-initio code based on wavelets is thus optimal to calculate electronic properties of big inhomogeneous systems such as found in nanoscience or biology.

At present, a stable and robust version of such code is ready, distributed with GNU-GPL license and integrated in ABINIT v. 5.5.x. The systematicity of the basis set together with the massive optimization of the operations performed make this code very fast and precise, with excellent efficiency on parallel computers. The properties of the basis functions are also well-suited for developing an *O(N)* code, which is one of the perspective for future developments.

During this presentation we will present the main features of the code, and we will show how this basis set can be used for efficient and reliable electronic structure calculations.

Modeling the localized-to-itinerant electronic transition in the heavy Fermion system CeIrIn$_5$

Kristjan Haule

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Within the ab-initio calculation we address the crossover from the localized to itinerant state of the heavy Fermion material CeIrIn$_5$. The temperature evolution of the one electron spectra and the optical conductivity is predicted from first principles. The buildup of coherence in the form of a dispersive many-body feature is followed in detail and its effects on the conduction electrons of the material is revealed. We find multiple hybridization gaps and link them to the crystal structure of the material. Our theoretical approach explains the multiple peak structures observed in optical experiments and the sensitivity of CeIrIn$_5$ to substitutions of the transition metal element and may provide a microscopic basis for the more phenomenological descriptions currently used to interpret experiments in heavy Fermion systems.

Spectral density functional: LDA+DMFT

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The local density approximation (LDA) for electronic structure calculations has been highly successful for non-correlated systems. The LDA scheme quite often failed, however, for strongly correlated materials containing transition metals and rare-earth elements with complicated charge, spin, and orbital ordering. Dynamical mean field theory (DMFT) in combination with the first-principle scheme (LDA+DMFT) can be a starting point to go beyond static density functional approximation and include effects of charge, spin and orbital fluctuations. The corresponding spectral density functionals give a theoretical background for self-consistent LDA+DMFT calculations in solids. Realistic approaches to different correlated electron problems such as half-metallic ferromagnetism and metal-insulator transition in transition metal oxides will be discussed.

Ab-initio finite-temperature excitons

Andrea Marini

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The ab-initio description of the excitonic states, obtained by solving the Bethe-Salpeter equation (BSE) of many-body perturbation theory, constitutes a well-established approach to interpret the photoexcited properties of bulk materials, surfaces, nanostructures and organic/bio-molecules [1]. In the standard approach, however, the BSE is solved assuming the atoms frozen in their crystallographic positions, thus neglecting the effect of lattice vibrations [2]. As a consequence excitons turn out to be insensitive to the temperature T and with an infinite lifetime, in stark contrast with the experimental evidence. A paradigmatic example is given by bulk semiconductors, like silicon and hexagonal BN, where it is a well-known fact that the absorption line position, width and intensity show a clear T dependence [2]. In the frozen-atom BSE this dependence is not described at all and, even in the $T \rightarrow 0$ limit, the calculated absorption spectra is commonly convoluted with some artificial, ad-hoc numerical broadening function chosen to yield the best agreement with experiment. More generally the finite temperature non-radiative damping, and the energy and optical strength renormalization, define the quantum efficiency of the excitons as photo-emitters, a key parameter in devising materials for optoelectronic applications.

In this talk I will show how to solve, in a fully ab-initio manner, the Bethe-Salpeter equation including the coupling with the lattice vibrations. The picture of the excitons obtained within a frozen-atom approximation turns out to be deeply modified by the exciton-phonon coupling, either at zero and finite temperature. Large zero-point motion effects are found in hexagonal BN where the lowest exciton binding energy is reduced by $\approx 30\%$. In the finite temperature regime, the BSE describes a wealth of new physical features. Excitons acquire a non-radiative lifetime (otherwise infinite in the frozen-atom BSE) and undergo bright to dark (and vice versa) transitions. Consequently the basic definitions of optical brightness and optical efficiency will be shown to be strongly temperature dependent. Finally, the finite temperature optical spectra of Si and hexagonal BN are reproduced in excellent agreement with the experimental results.

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Compensation mechanisms and functionality of perovskite interfaces

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Charge imbalance at oxide interfaces (IF) can drive novel behavior unanticipated in the respective bulk compounds. For example interfaces between the two simple nonmagnetic band insulators $LaAlO_3$ and $SrTiO_3$ were reported to be conducting [1], magnetic [2] and even superconducting [3]. Density-functional theory calculations including a Hubbard U reveal that the charge mismatch at this and also at the $LaTiO_3$/$SrTiO_3$ interface is accommodated by charge disproportionation (Ti^{3+} and Ti^{4+}), orbital ordering (d_{xy}) and slight preference for an antiferromagnetic alignment of the Ti^{3+} spins [4,5]. An enhanced complexity with respect to orbital occupation is observed at the $LaVO_3$/$SrTiO_3$ interface. Furthermore, I will focus on the effect of lattice relaxations on charge order as well as on the influence of the surface on the interfacial electronic properties.

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Lanczos-based cluster methods for strongly correlated electron systems

Michael Potthoff

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Phase diagrams and elementary excitation spectra of strongly correlated electron systems can be studied by solving the problem numerically for a finite cluster, which is first cut out of the infinite lattice and then embedded again. Here we discuss cluster approaches where the isolated cluster is treated with the Lanczos method at T=0 while the embedding is done within the framework of the self-energy-functional approach. The one-dimensional Hubbard model is considered for a benchmark of the method. We test different clusters, with and without bath degrees of freedom, in different topologies and with different sets of variational parameters. In particular, we study the role of bath sites for the description of excitation properties and as charge reservoirs for the description of filling dependencies. For the two-dimensional case, first results for the metal-insulator and the magnetic phase transition are presented.

Optical spectrum of water: many-body perturbation theory meets molecular dynamics

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We present calculations of the electronic levels and optical spectra of liquid water in the framework of many-body Green's function formalism. Snapshots taken from molecular dynamics simulations are used as input geometries to calculate electronic levels and absorption spectra, and the results are averaged over the different configurations. The electronic states are obtained within the so called "GW" approximation to take fully into account exchange and correlations effects. The optical absorption spectra are calculated by solving the Bethe-Salpeter equation, which includes excitonic effects by explicitly introducing the electron-hole Coulomb interaction. The spectra are strongly modified by many-body effects, both in peak energies and in lineshapes. Finally, we discuss how to calculate the optical properties of large scale systems, using many-body perturbation theory combined with quantum-mechanics/molecular-mechanics. We show how to include quasi-particle and excitonic effects for the calculation of optical properties in a QM/MM scheme. We apply this scheme to indole in water solution. We observe that the solvent induces a red shift in the first spectral peaks of indole, in agreement with the experiments.

Continuous time QMC methods:
Applications for DMFT and beyond

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We review the current situation in the novel numerical technique for correlated fermionic systems: continuous-time quantum Monte Carlo (ct-qmc) for Fermions. This family of numerically exact solvers is based on a stochastic series expansion for the partition function in the interaction representation. The method is particularly applicable for multi-band, time-dependent correlations since it does not invoke the Hubbard-Stratonovich transformation. We will describe how this method can be employed for DMFT calculations of realistic models with strong localized correlations. Practical examples will be given. The talk will also touch recently developed dual-Fermion approach, that is an extension of the DMFT scheme developed to take the non-local part of correlations into account.

Are self-energies local?
Insights from LDA+DMFT and GW+DMFT

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I will discuss recent progress in applications of dynamical mean-field theory for electronic structure calculations of strongly correlated materials. The spectral density functional approach will be reviewed which provides a formal foundation for such a theoretical framework. Applications will cover energetics and spectroscopy of Mott-Hubbard insulators, high temperature superconductors, as well as some actinide systems. I will also discuss some recent developments of GW+DMFT where the convergence of electronic self-energies in real-space will be tracked for metals and semiconductors.

Wannier interpolation and its application to the calculation of anomalous Hall conductivity

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The intrinsic anomalous Hall conductivity (AHC) in ferromagnets depends on subtle spin-orbit-induced effects in the electronic structure, and recent ab-initio studies found that it was necessary to sample the Brillouin zone at millions of k-points to converge the calculation. I will present an efficient first-principles approach based on Wannier functions for computing this and other properties of metals demanding a very dense k-point sampling. Two alternative strategies to the evaluation of the AHC will be discussed. The first is a Fermi-sea calculation, whereby the AHC is expressed as the integral of the k-space Berry curvature over the occupied portions of the Brillouin zone. The second is a Fermi-surface reformulation, based on evaluating the Berry-phase accumulated by the Bloch states as they are transported around closed loops on the Fermi-surface. Illustrative calculations are performed for Fe, Co and Ni.

Optimization of quantum Monte Carlo wave functions by energy minimization

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We present a simple, robust and highly efficient method for optimizing the parameters of many-body wave functions by energy minimization in quantum Monte Carlo calculations. Using a strong zero-variance principle, the optimal parameters are determined by diagonalizing the Hamiltonian matrix in the space spanned by the wave function and its derivatives [1-2]. We apply this method to obtain accurate multideterminant Jastrow-Slater wave functions for atomic and molecular systems, where the Jastrow parameters, the configuration state function coefficients, the orbital coefficients and the basis function exponents are simultaneously optimized. This allows us to reach near chemical accuracy on the dissociation energies of the first-row diatomic homonuclear molecules [3].

[1] J. Toulouse and C. J. Umrigar, J. Chem. Phys. **126**, 084102 (2007)
[2] C. J. Umrigar, J. Toulouse, C. Filippi, S. Sorella, and R. G. Hennig,
    Phys. Rev. Lett. **98**, 110201 (2007)
[3] J. Toulouse, C. J. Umrigar, in preparation

Orbital order in the frustrated spinel ZnV_2O_4

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The orbital order in the spinel ZnV_2O_4 is presently a subject of considerable debate. In this system the V ions are in a spin-1 state characterized by double occupancy of the triply degenerate t_{2g} orbitals. These partially filled t_{2g} orbitals leave the orbital degrees of freedom unfrozen opening up the possibility of orbital order. Moreover, the V-sites in the cubic spinel structure form a pyrochlore lattice, which gives rise to frustrated antiferromagnetic interactions among these sites. I will discuss the complex behavior of this system in the framework of ab initio electronic structure calculations and effective model considerations and show that it is the spin-orbit coupling along with electronic correlations which play a significant role in determining the orbital structure in this material.

The GW space-time formalism at finite temperature for metallic systems

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We present the extension to finite temperatures of the space-time formulation of the GW approach to electronic structure. The treatment of the time and frequency dependence of different quantities is described in detail, as it differs strongly from the standard real frequency reciprocal space approaches; in particular, the polarizability, the dynamically screened interaction, and the self-energy must all be considered on a finite length interval in imaginary time and using the Matsubara formalism. The dielectric properties of metallic systems in this context are clarified. We apply the formalism to metallic systems and discuss perspectives, in particular for electron transport in nanostructures including correlation effects.

Recent progress in auxiliary-field electronic structure methods

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We have been developing an auxiliary-field quantum Monte Carlo method for many-body electronic structure simulations. The method takes the form of a linear superposition of independent-electron calculations in fluctuating external fields. "Entanglement" of the different field configurations leads to random walks in the space of mean-field solutions. Each random walk stream resembles a density-functional theory (DFT) calculation in fluctuating local external potential. We formulate an approximate constraint on the random walk paths to control the sign/phase problem. Often simple mean-field solutions taken directly from DFT or Hartree-Fock calculations have been used as the constraining wave function. This approach has performed well in close to 100 molecular and solid systems tested to date. I will discuss briefly the method and applications, and report on our recent effort toward systems of larger sizes and stronger correlation effects, and excited states.

In collaboration with W. A. Al-Saidi, Henry Krakauer, Hendra Kwee, and Wirawan Purwanto

Posters

Band structure anomaly of chalcopyrite semiconductors CuGaX$_2$ vs. AgGaX$_2$ (X=S, Se) and their alloys

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Due to the important technological applications in nonlinear optics, light-emitting diodes, and solar cells, the I-III-VI2 ternary semiconductors (AgGaS$_2$, AgGaSe$_2$, CuGaS$_2$ and CuGaSe$_2$) and their alloys have attracted much attention recently. As a result of the added chemical and structural freedom of these compounds relative to their II-VI analogs (CdZnS$_2$, CdZnSe$_2$, ZnS and ZnSe), they exhibit some abnormal chemical trends. For example, these chalcopyrite compounds not only have large downward shifts in the band gap relative to their binary analogs, but the band gaps of AgGaX$_2$ (2.65 and 1.81 eV for X=S and Se) are also larger than the corresponding CuGaX$_2$ (2.43 and 1.68 eV for X=S and Se), despite that the lattice constants of AgGaX$_2$ are larger than for CuGaX$_2$. Furthermore, the experimental studies show that the Ag$_x$Cu$_{1-x}$GaX$_2$ alloys have large band gap bowing, especially for the sulfides, which contradicts to the previous prediction based on phenomenological model.

Using first-principles methods, we calculated the structural and electronic properties of these ternary semiconductors and their disordered alloys [1]. We found that (i) besides the upward shift of the VBM states caused by *p-d* coupling between group I and VI atoms, the wavefunction localization of the CBM states at the group III site also plays an important role on the band gap reduction of the chalcopyrites relative to their binary analogs. (ii) Because of the higher *d* level and smaller size, Cu compounds CuGaX$_2$ have stronger *p-d* coupling than AgGaX$_2$, thus, the valence band offsets between common-anion pairs CuGaX$_2$/AgGaX$_2$ are large and negative (i.e., CuGaX$_2$ has higher VBM than AgGaX$_2$), opposite to the case in their II-VI analogs. This is also the origin why the band gap of AgGaX$_2$ is larger than CuGaX$_2$. (iii) The valence band offsets between MIGaS$_2$/MIGaSe$_2$ (MI=Cu, Ag) are significantly smaller than their II-VI analogs, because the *p-d* coupling decreases the *p* level energy difference of S and Se. (iv) The large band offset and lattice mismatch between CuGaS$_2$/AgGaS$_2$ give rise to the large band gap bowing of Ag$_x$Cu$_{1-x}$GaS$_2$ alloy. (v) The bowing parameters for the common-anion alloys are larger than the common-cation alloys, following the same trend as the valence band offsets and lattice mismatch. Our calculated results are in good agreement with experimental observations.

[1] S. Chen, X. G. Gong, and S.-H. Wei, Phys. Rev. B **75**, 205209 (2007)

Study of spin-charge separation for next-neighbor Coulomb interaction in TTF-TCNQ

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The photoemission spectrum of the quasi one-dimensional organic metal TTF-TCNQ can be described qualitatively using an effective *t-U* Hubbard model. Using cluster perturbation theory (CPT) calculations, we can calculate angular-resolved spectral functions with high resolution and resolve signatures of spin-charge separation.

Experiments and theoretical calculations to obtain realistic parameters for TTF-TCNQ suggest, however, a hopping parameter *t* which is smaller by a factor of two than in the effective *t-U*-model. In addition it turns out that the next-neighbor Coulomb repulsion *V* cannot be neglected. We observe that *V* effectively doubles the bandwidth but at the same time the spectral weight of the holon-band spreads and the simple spin-charge separation picture is lost. To study this transition we perform kCPT computations which are similar to CPT but computationally less demanding at the expense of some resolution in *k*-space. Moreover we study the nature of the dispersion in the *t-U-V*-model by calculating spin and charge correlation functions.

Order-*N* scaling in the full-potential
linearized augmented plane wave method

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Density functional theory codes based on the Full-potential Linearized Augmented Plane Wave (FLAPW) method have been highly successful due to their generality and wide applicability. In particular, in the field of surfaces, open structures and complex magnetic materials only few rivaling methods with similar precision are available. On the other hand, the FLAPW method is relatively computational expensive with a cubic scaling behaviour with system size limiting its applicability to smaller systems.

We will present our ideas to combine the Green function embedding method and the transfer-matrix formalism with the LAPW basis set to construct a computer code with a (roughly) linear scaling of the computational effort with system size. The total problem is decomposed into layers which can be calculated individually and are joint together with the help of the embedded Green function technique.

Understanding correlations in vanadium oxide from first principles

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Vanadium dioxide is a prototype material for the discussion of correlation effects in solids. First-principles density-functional theory does not describe the metal-insulator transition, whereas strongly correlated models reproduce the main features. Here we present a parameter-free GW calculation of VO_2 and show that correlation effects in the bandstructure of both the metallic and the insulating phases are correctly reproduced, provided that quasiparticle energies and wavefunctions are calculated self-consistently. Our calculations explain the satellite in the photoemission spectrum of the metal as due to a plasmon resonance in the energy-loss function and show that this feature disappears in the insulator.

Transforming nonlocality into frequency dependence: a shortcut to spectroscopy

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Measurable spectra are theoretically very often derived from complicated many-body Green's functions. In this way, one calculates much more information than actually needed. Here we present an in principle exact approach to construct effective potentials and kernels for the direct calculation of electronic spectra. In particular, the potential that yields the spectral function needed to describe photoemission turns out to be dynamical but *local* and *real*. As example we illustrate this "photoemission potential" for sodium and aluminium, modeled as homogeneous electron gas, and discuss in particular its frequency dependence stemming from the nonlocality of the corresponding self-energy. We also show that our approach leads to a very short derivation of a kernel that is known to well describe absorption and energy-loss spectra of a wide range of materials.

Continuous time quantum Monte Carlo method for multiorbital strongly correlated systems

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We propose a numerically exact scheme to calculate spectral and magnetic properties of correlated systems. The scheme employs the weak-coupling determinantal continuous time quantum Monte Carlo method for the solution of the quantum impurity problem. This approach can treat multiorbital impurity models including Coulomb interaction of the most general form. We show a possibility to calculate magnetic susceptibilities of a single-spin Kondo impurity embedded into different environments: an ultrasmall grain, the Anderson model, corresponding to a lattice with random on-site energy levels, and a two-dimensional lattice, where the density of states has a van Hove singularity.

The realistic five-band model for transition metal atom d-shells with full Coulomb interaction vertex as a Kondo impurity in a metal matrix has been calculated. In order to calculate properties of correlated solids, the continuous time quantum Monte Carlo method is used as an impurity solver within the dynamical mean-field theory. The metal-insulator phase transition for two and three anisotropic orbitals on the Bethe lattice with spin-flip interactions is considered. The method is applied to a real correlated solid, namely strontium ruthenate Sr_2RuO_4. The $4d$-t_{2g} orbitals of Ru were considered as an effective three-band model. We investigated the role of non-diagonal terms in the interaction part of the Hamiltonian, related to spin flip and pair hopping interactions.

Fermiology of cuprates from first principles:
From small pockets to the Luttinger Fermi surface

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Realistic electronic-structure calculations for correlated Mott insulators are notoriously hard. Here we present a multiconfiguration quantum-chemical scheme that adequately describes strong correlation effects involving Cu-3d and O-2p electrons in layered cuprates. In particular, the O-2p states giving rise to the Zhang-Rice band are explicitly considered in our approach. Renormalization effects due to nonlocal spin interactions are also treated consistently. We show that the dispersion of the bands observed in photoemission is reproduced with quantitative accuracy. Additionally, the evolution of the Fermi surface with doping follows directly from our ab-initio data, for both hole and electron doped cuprates. Our results thus open a new avenue for the first-principles investigation of the electronic structure of correlated Mott insulators.

A computational study of electronic and optical properties of superconducting materials using density functional theory

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The present work is an overview of the electronic and optical properties of a selection of superconducting materials carried out using first principles density functional calculations as implemented in the electronic structure package, CASTEP. The structure, bonding, electronic band structure, density of states, charge-density and optical properties are being considered for the materials at ambient and at higher pressures. The results and discussion are illustrated in the poster.

Maximally-localized Wannier functions within the full-potential linearized augmented plane-wave method applied to transport in thin metallic wires

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We report on the implementation of a transport scheme for one-dimensional systems based on maximally-localized Wannier functions (MLWFs) constructed within the full-potential linearized augmented plane-wave (FLAPW) method. We describe the details of the MLWFs construction from the FLAPW wavefunctions including the case of spin-orbit coupling and choose a monoatomic Pt chain as a model system.

For the calculation of ballistic transport we apply the Greens function method. The Hamiltonian of the system including a scattering region attached to semi-infinite leads is constructed from the MLWFs which serve as a localized basis set. The open boundary problem is solved by replacing the leads by self-energies obtained via the decimation technique. From the Greens function we can immediately calculate the conductance of the system.

As a first application of the approach, we study the transition from the contact to the tunneling regime in thin Pt wires with a stretched bond.

Bath-symmetries and hybridization sum-rules for CDMFT and DCA

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In the Hamiltonian formulation of CDMFT and DCA, the point symmetries of the cluster imply symmetries of the hybridization, which can substantially reduce the number of independent parameters to fit the bath Green function. We review these symmetries and derive general sum-rules for the hybridizations, which (i) allow to check the quality of a fit using a finite set of bath sites and (ii) imply what hybridizations vanish. As examples we discuss calculations for the Hubbard model in one-dimension and for 2x2 clusters.

Dynamical vertex approximation:
a step beyond dynamical mean-field theory

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We have developed a new diagrammatic approach, coined "Dynamical Vertex Approximation" (DΓA), with the aim of going beyond dynamical mean field theory for strongly correlated systems, by including the effects of long-range spatial correlations. Without resorting to any finite-size cluster scheme, DΓA allows us to compute momentum dependent self-energies (and spectra), whose expressions are diagrammatically constructed starting from the two-particle irreducible local vertex. Therefore, DΓA naturally applies for studying effects of magnetic fluctuations with large correlation length in strongly correlated systems, such as the Hubbard model. Specifically, we analyze the interplay between antiferromagnetic fluctuations and the Mott metal-insulator transition in three dimensions and the formation of a pseudogap in two dimensions. The diagrammatic nature of DΓA, moreover, should allow for a generalization to the more realistic case of multi-band Hamiltonians.

[1] A. Toschi, A. Katanin, and K. Held, Phys. Rev. B **75**, 045118 (2007)

Exchange interactions in heavy fermion superconductors

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The exchange interactions of several Ce and Pu based heavy Fermion materials will be calculated based on the combination of local density approximation and dynamical mean field theory. The results will be discussed in connection to the superconductivity in those systems

All electron calculations of electronic transport: Applications to magnetic tunnel junctions

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The theoretical description of electron transport imposes a formidable problem of quantum physics. The difficulties arise on very different levels, (i) the description of non-equilibrium processes in a many-body system, (ii) to include the properties of real materials and (iii) to include the geometrical constraints present in the different setups. While the formulation of the single-particle current is a trivial exercise, calculating the electronic current in a many-particle system is extremely challenging. Recently, the calculation of conductances within the density functional theory became feasible. Taking the DFT single particle description literally, many groups implemented various schemes to calculate the current through some active region sandwiched between two semi-infinite electrodes. The broken periodicity of these setups with the attached leads made the calculation of open systems necessary, a task most often solved in a tight-binding formulation.

Important advances have been made possible by employing the non-equilibrium Keldysh Green function method to include effects due to an applied bias putting the system into a non-equilibrium state. These calculations within the DFT include screening and charge transfer effects and other induced changes on the electronic structure. Most codes used in this field employ a localized basis which supports a partitioning of the Hamiltonian into separate contributions arising from the leads and the interface region. Motivated to describe electronic transport in the context of an all-electron full-potential scheme, we implemented the Green-function embedding formalism within the framework of the full-potential linearized augmented plane wave (FLAPW) method. This approach allows the calculation of the embedded Green function of the finite scattering region with the correct boundary conditions of attached semi-infinite leads, which appear as additional non-local potentials in the transport calculations. The well-known formulas to calculate the coherent current using the Landauer formula and the incoherent one using Bardeen's formula are expressed in terms of the embedded Green function.

We applied our Green function embedding method to two different magnetic tunnel junctions. First we will discuss the Fe/MgO/Fe systems which attracted much attention recently and became the most promising candidate for high TMR values. While Al_2O_3 barriers studied extensively in the past only provided TMR values as low as 20%, theoretical investigations based on first-principles calculations predicted high TMR values for perfectly ordered (100) oriented single-crystalline Fe/MgO/Fe junctions. A breakthrough was achieved in 2004 with room-temperature values of about 230% using these theoretically suggested tunnel junctions with a MgO barrier. Since then several further record high values have been reported by several Japanese groups approaching the high TMR values that have been theoretically predicted. In our calculations we modified the chemical composition of the interface and study the effect the spin-polarization of the electronic transmission. In particular, we present Fe/X/MgO/Fe tunnel junctions in which additional layers of X=V,Cr,Co or Ag have been added. We will demonstrate how these modifications of the metal/insulator interface affect the tunneling properties and how these correlate with the changes of the electronic structure. Additionally, we show the unfavorable effect of the formation of an FeO layer on the TMR stressing the need to prepare high-quality junctions for devices.

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