



# Strong Correlation from First Principles

Monastery Seon, Bavaria, Germany

August 30 – September 2, 2011

## Organizers

Silke Biermann (Ecole Polytechnique, Palaiseau)

Patrick Rinke (Fritz Haber Institute, Berlin)

## -Final Report-



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The workshop Strong Correlation from First Principles (SC1p) was held at Kloster Seeon from August 30 to September 2, 2011. The first-principles description of strongly correlated materials (typically materials containing partially filled d- or f-shells) is one of the great challenges in condensed matter physics. Strongly correlated materials such as complex oxides are becoming evermore important for technological applications, while simultaneously offering a plethora of physical phenomena (e.g. high temperature superconductivity) that continue to challenge our current understanding. Many disjointed approaches to tackle the problem are currently being pursued in the electronic structure community, by many-body theorists and quantum chemists. The SC1p workshop brought together 45 scientists from different communities who actively debated the very foundations of the challenges that lie ahead. The momentum generated by SC1p will be carried forward to a symposium with the same name at the March Meeting of the German Physical Society in Berlin in 2012 that has already been approved. The success of the SC1p workshop this year makes us confident that a series of workshops dedicated to the first principles treatment of strong correlations could develop. This series could provide the synergy to shape the future development in this important research area and would provide a unique opportunity to promote this emerging field in the European research landscape.

45 participants from leading international groups attended the workshop and presented 16 oral contributions (11 invited and 5 contributed talks) as well as 24 posters. Two overview talks on the first evening introduced the subject from two different angles. Over the course of the next three days invited experts presented their current results and insights into the topic. We had deliberately limited the time for presentations to 25min and reserved 20min for discussion after each presentation. For contributed talks the partition was 15min and 10min. This turned out to be an excellent idea, because it really encouraged lively discussion after each talk that continued into the coffee, lunch and dinner breaks. It also gave younger researchers the opportunity to participate in the discussions and to ask questions, which is often not the case at large conferences that permit only a limited number of questions that are then taken up by established scientists in the field.

Since two different communities with different philosophies and viewpoints came together in this workshop the discussions were very insightful for all participants. This was also the motivation for the round table discussion that took place Thursday morning. We had realized that many participants had submitted abstracts on the same materials system (transition metal monoxides). To spare the audience from having to hear the same introductory material several times, we decided to pool the presentations into one moderated round table, in which each speaker was given 5min to introduce the most important results or open problems. The ensuing discussion was active and productive (also thanks to the excellent moderation of G. Sawatzky) and makes us confident, that this format might be a viable alternative to the usual presentation style at scientific conferences.

Kloster Seeon in Bavaria provided the perfect venue for the workshop. The local organization at Kloster Seeon was smooth and extremely professional. The technical facilities in the conference room were state-of-the-art and easy to use. Posters were mounted in the coffee area and were on display for the whole duration of the workshop. This facilitated active discussions in front of the posters well beyond the time of the poster session on Wednesday evening. The fact that accommodation and conference facilities share the same premise at Kloster Seeon and that lunch and dinner were also served on site provided an informal atmosphere for stimulating discussions and gave conference attendants ample time to exchange ideas.

# Program

## Tuesday, 30 Aug.

19:00 - 20:15	Dinner
20:15 - 20:30	Welcome
20:30 - 20:55	Antoine Georges (CPHT-Ecole Polytechnique): <i>Strong Electronic Correlations: what they are and how to treat them</i>
20:55 - 21:15	Discussion
21:15 - 21:40	Lucia Reining (LSI, Ecole Polytechnique): <i>Correlation: coupling of excitations</i>
21:40 - 22:00	Discussion

## Wednesday 31 Aug.

09:00 - 09:25	Alexander Lichtenstein (University of Hamburg): <i>Strong Electronic Correlations in real materials</i>
09:25 - 09:45	Discussion
09:45 - 10:05	Hong Jiang (Peking University): <i>Electronic band structures of d- and f-electron systems from GW@LDA+U perspective</i>
10:05 - 10:20	Discussion
10:20 - 10:50	Coffee Break
10:50 - 11:10	Jan Kuneš (Institute of Physics, Praha): <i>Multireference Local States in Solids with Dynamical Mean-Field Theory</i>
11:10 - 11:25	Discussion
11:25 - 11:40	Bernard Amadon (CEA – Département de Physique): <i>An LDA+DMFT implementation in the Projector Augmented Wave: Applications to f electrons systems</i>
11:40 - 11:50	Discussion
12:00	Lunch
14:00 - 14:25	Hardy Gross (MPI Halle): <i>Density-matrix functional theory of strongly correlated solids</i>
14:25 - 14:45	Discussion
14:45 - 15:10	Xinguo Ren (Fritz-Haber-Institut): <i>Towards a general-purpose first principles method: a critical assessment of the random phase approximation and beyond</i>
15:10 - 15:30	Discussion
15:30 - 16:00	Coffee Break
16:00 - 16:15	David Jacob (MPI Halle): <i>COHSEX+OCA and COHSEX+DMFT for nanoscopic conductor</i>
16:15 - 16:25	Discussion
16:25 - 16:40	Loig Vaugier (CPHT-Ecole Polytechnique): <i>Hubbard U from the constrained Random Phase Approximation (cRPA) within a full-potential linearized augmented plane wave approach: Trends for 3d and 4d transition metal perovskites</i>
16:40 - 16:50	Discussion
17:00	Poster session
19:00	Dinner

<b>Thursday 01 Sept.</b>	
09:00 - 09:20	Sokrates Pantelides (Vanderbilt University): <i>Density functional theory for d-electron systems - Are there really strong correlations?</i>
09:20 - 09:35	Discussion
09:35 - 09:50	Cyril Martins (CPHT-Ecole Polytechnique): <i>Spin-orbital polarization in paramagnetic transition metal oxides: <math>Sr_2IrO_4</math> versus <math>Sr_2RhO_4</math></i>
09:50 - 10:00	Discussion
<b>10:00 - 10:30</b>	<b>Coffee Break</b>
10:30 - 12:00	Roundtable discussion: Transition metal monoxides Chairman: G. Sawatzky Contributors: Kuneš, Jiang, Gatti, Schroen, Thunstroem, Guzzo, Lichtenstein and whoever wants to say something on transition metal monoxides (please contact S. Biermann) a) Short general introduction -15 min- to MnO, NiO, FeO, CoO by the Chairman b) Every speaker has max. 3 to 4 slides and max. 5 minutes
<b>12:00</b>	<b>Lunch</b>
Excursion	
<b>20:00</b>	<b>Dinner</b>
<b>Friday 02 Sept.</b>	
09:00 - 09:25	George Sawatzky (UBC – Departement Chemistry): <i>Effective Coulomb and multiplet interactions in correlated electron systems: Experimental determinations and importance of non uniform polarizability</i>
09:25 - 09:45	Discussion
09:45 - 10:10	Philipp Werner (ETH Zürich): <i>Dynamical screening in correlated electron materials</i>
10:10 - 10:30	Discussion
<b>10:30 - 11:00</b>	<b>Coffee Break</b>
11:00 - 11:15	Michele Casula (UPMC Paris): <i>Satellites and large doping- and temperature dependence of electronic properties in hole-doped <math>BaFe_2As_2</math></i>
11:15 - 11:25	Discussion
11:25 - 11:50	Giorgio Sangiovanni (Vienna University of Technology): <i>Dynamical Vertex Approximation for Nanoscopic Systems</i>
11:50 - 12:10	Discussion
<b>12:15</b>	<b>Lunch</b>
<b>13:30</b>	<b>Departure</b>

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# Strong Electronic Correlations: what they are and how to treat them

Antoine Georges

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From copper-oxide superconductors to rare-earth compounds, materials with strong electronic correlations have focused enormous attention over the last few decades.

In this introductory talk, I will emphasize that electronic correlations are primarily manifestations of single-atom physics in the solid-state context. For this reason, the classic paradigm of solid-state physics, in which a solid is viewed as a gas of (almost) independent particles, must be seriously revised for strongly correlated materials. Theoretical descriptions that use this paradigm, even when formally exact, have a hard time grasping the physics of such materials.

Instead, a description accounting for both atomic-like excitations in real-space and quasiparticle excitations in momentum space is requested. I will briefly review how Dynamical Mean-Field Theory -an approach that has led to significant advances in our understanding of strongly correlated materials- gets us closer to this goal.

## Correlation: coupling of excitations

Giovanna Lani<sup>1,4</sup>, Pina Romaniello<sup>2,4</sup>, Matteo Gatti<sup>3,4</sup>, Lucia Reining<sup>1,4</sup>

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3. *Dpto. Física de Materiales, Universidad del País Vasco, San Sebastián, Spain*
4. *European Theoretical Spectroscopy Facility*

To describe electronic correlations is one of the big challenges of condensed matter theory. In this talk we will discuss correlation from the point of view of many-body perturbation theory, starting from the GW approximation [1] and going beyond. We will focus on the interpretation of correlation effects as due to the coupling of different excitations. In GW, this is achieved by the screened Coulomb interaction  $W$ ; indeed it is simply the screening of the Coulomb interaction that makes the difference between Hartree-Fock and GW. Static screening gives rise to a renormalization of energies. Dynamical screening contains additional excitations that can be seen as satellites in photoemission spectra. Beyond GW, for example the T-matrix approximation [2] privileges other kinds of excitations. The main point of this talk will be to put different approaches on the same footing and to compare their content, limitations and promises. Systems used for illustration will include models, simple semiconductors, carbon nanostructures and transition metal oxides.

[1] L. Hedin, Phys. Rev. **139**, A796 (1965).

[2] see e.g. L. P. Kadanoff and G. Baym, *Quantum Statistical Mechanics* (W.A. Benjamin Inc., New York, 1964).

# Strong Electronic Correlations in real materials

Alexander Lichtenstein

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Effects of electron interactions in different materials, including superconducting oxides and transition metal magnetic impurity on copper and Graphene will be introduced. Modern density functional theory describe well the ground state properties but not the spectroscopy of strongly correlated magnetic materials with transition or rare-earth elements. We have investigated the possibility to go beyond simple dynamical mean field theory which allowed to analyzed non-local correlations effects. Prospects of realistic description of local multi-orbital correlation effects for Co-atom will be discussed.

# Electronic band structures of $d$ - and $f$ -electron systems from the $GW@LDA+U$ perspective

Hong Jiang

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The accurate first-principles description of  $d$ - and  $f$ -electron systems is currently regarded as one of the great challenges in condensed matter physics due to the simultaneous presence of itinerant (delocalized) and highly localized states and interactions between them. Density-functional theory (DFT) in the local-density approximation (LDA) proves to be inadequate for  $d/f$ -electron systems due to the severe self-interaction (delocalization) error. The simplest extension that can overcome the major failure of LDA is by introducing a local Hubbard like correction (LDA+U), which, however, treats itinerant states still at the LDA level. Many-body perturbation theory in the GW approach offers both a quasi-particle perspective (appropriate for itinerant states) and an exact treatment of exchange (appropriate for localized states). The combination of GW with LDA+U ( $GW@LDA+U$ ) is therefore promising for  $d/f$ -electron systems. In this talk, I will present a systematic investigation of the  $GW@LDA+U$  approach, as implemented in our newly developed all-electron GW code FHI-GAP (Green's function with Augmented Planewaves) [1], for a series of prototypical  $d$ - and  $f$ -electron systems including later transition metal oxides [2], lanthanide oxides [3] and actinide oxides [4]. We observed good agreement between the GW density of states and experimental spectra using  $U$  determined by the constrained DFT approach. All main features found in experimental band gaps of the lanthanide sesquioxide series ( $Ln_2O_3$ ) are well reproduced by our approach. Consistent with other GW approaches, the satellite structure in the photoemission spectroscopy of late transition metal oxides is still missing, and the binding energy of occupied  $d/f$ -states tends to be underestimated. We also compare  $GW@LDA+U$  to other variants of GW approaches as well as dynamical mean-field theory to illuminate pros and cons of different approaches.

- [1] H. Jiang, R. Gomez-Abal, X. Li, H. Jiang, C. Meisenbichler, C. Ambrosch-Draxl, M. Scheffler, in preparation (2011)
- [2] H. Jiang, R. Gomez-Abal, P. Rinke, and M. Scheffler, Phys. Rev. B 82, 045108 (2010)
- [3] H. Jiang, R. Gomez-Abal, P. Rinke, and M. Scheffler, Phys. Rev. Lett. 102, 126403 (2009)
- [4] H. Jiang, P. Rinke and M. Scheffler, in preparation (2011).

# Multireference Local States in Solids with Dynamical Mean-Field Theory

J. Kuneš

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The term correlated in general denotes a system that cannot be described as a 'product' of its components. In the electronic context this means that a state is not close to a Slater determinant. We will discuss the application of the dynamical mean-field theory (DMFT) to a subset of the strongly correlated materials, in which the local reference state has a non-trivial quasi-degeneracy. As examples we will use the pressure-induced spin transition in MnO [1] and Fe<sub>2</sub>O<sub>3</sub> [2] or the temperature-induced spin transition in LaCoO<sub>3</sub> [3]. In these cases the degeneracy involves the high-spin and low-spin multiplets of the corresponding valence states. Another example is provided by the valence transition in elemental Yb [4], where the degeneracy takes place between the  $4f^{13}$  and  $4f^{14}$  charge states of the  $4f$  shell. The quantum dynamics of the correlated atoms as obtained from the auxiliary impurity problem of DMFT will be discussed in detail.

- [1] J. Kuneš *et al.*, Nature Materials **7**, 198 (2008);
- [2] J. Kuneš *et al.*, Phys. Rev. Lett. **102**, 146402 (2009);
- [3] J. Kuneš and V. Křápek, arXiv:1103.2249;
- [4] E. R. Ylvisaker *et al.*, Phys. Rev. Lett. **102**, 246401 (2009).

# An LDA+DMFT implementation in the Projector Augmented Wave: Applications to $f$ electrons systems.

Bernard Amadon

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The combination of density functional theory in the local density approximation (LDA) and dynamical mean field theory (DMFT) [1] has been successful to describe localized or delocalized correlated electrons in condensed matter physics [2]. However, the accurate calculations of structural properties in this framework are scarce and drastic simplifications are sometimes made, such as the atomic sphere calculation (ASA) or the lack of self-consistency over electronic density. We present an implementation of the LDA+DMFT with the self-consistency over both the local green function and the local density. The implementation [3,4] is based on a plane wave/projector augmented wave implementation in ABINIT [5]. In order to have an accurate calculation of total energy, a careful benchmark with LDA+U and previous results obtained with LDA+DMFT on  $f$ -electrons systems is done. Applications on structural properties of  $f$  electrons systems are given.

- [1] A. Georges, G. Kotliar, W. Krauth, and M. J. Rozenberg *Rev. Mod. Phys.* **68**, 13 (1996).
- [2] G. Kotliar et al., *Rev. Mod. Phys.* **78**, 865 (2006).
- [3] B. Amadon, F. Lechermann, A. Georges, F. Jollet, T.O. Wehling and A.I. Lichtenstein *Phys. Rev. B* **77** 205112 (2008)
- [4] B. Amadon, [cond-mat/1101.0539] unpublished.
- [5] X. Gonze et al., *Comput. Phys. Commun.* **180**, 2582 (2009).

# Density-matrix functional theory of strongly correlated solids

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Systems with strong correlations, such as Mott insulators and stretched H<sub>2</sub>, cannot be described correctly with standard xc functionals in Kohn-Sham density-functional theory. In this communication we will demonstrate, that reduced-density-matrix-functional theory (RDMFT) represents a viable alternative to handle such strongly-correlated systems. Employing approximate functionals for the RDMFT xc energy and minimizing the total energy with the appropriate constraints ensuring N-representability of the one-body RDM, we present results for molecules [1] and periodic bulk insulators, including Mott insulators [2], as well as non-collinear magnetic phases of the uniform electron gas [3]. Finally we develop a novel approach [4] to extract spectral information, ultimately the spectral function of extended solids, from RDMFT. The calculated results turn out to be in excellent agreement with experiment.

- [1] N.N. Lathiotakis, S. Sharma, J.K. Dewhurst, F.G. Eich, M.A.L. Marques, E.K.U. Gross, *Phys. Rev. A* 79, 040501(R) (2009).
- [2] S. Sharma, J.K. Dewhurst, N.N. Lathiotakis, E.K.U. Gross, *Phys. Rev. B* 78, 201103(R) (2008).
- [3] F.G. Eich, S. Kurth, C.R. Proetto, S. Sharma, E.K.U. Gross, *Phys. Rev. B* 81, 024430 (2010).
- [4] S. Sharma, S. Shallcross, J.K. Dewhurst, E.K.U. Gross, *cond-mat/0912.1118*.

# Towards a general-purpose first principles method: a critical assessment of the random phase approximation and beyond

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Owing to its broad applicability and promise to overcome several intrinsic deficiencies of local/semilocal approximations to density functional theory (DFT), the random phase approximation for the ground-state correlation energy (cRPA) in combination with exact exchange (EX) has brought DFT one step further towards a general-purpose first principles method. This is largely due to three attractive features: the exact-exchange energy (EX) cancels the spurious self-interaction error present in the Hartree energy. The RPA correlation (cRPA) energy is fully non-local and includes long-range van der Waals (vdW) interactions automatically and highly accurately. Moreover, dynamic electronic screening is taken into account by summing up a sequence of ring diagrams to infinite order, which makes EX+cRPA applicable to small-gap or metallic systems. However, the standard RPA practice, i.e., evaluating both the EX and cRPA terms using Kohn-Sham orbitals from local/semilocal functionals, systematically underestimates bond strengths across a variety of systems. Two recent additions to cRPA have successfully ameliorated the underbinding problem: second-order screened exchange (SOSEX) [1,2] and renormalized single excitation corrections (RSE) [3]. From a diagrammatic point of view, SOSEX and RSE correspond to different types of many-body correlation terms that are, however, compatible with each other. In this work, we systematically benchmark the influence of SOSEX, RSE, and their combination on the atomization energies of the covalently bound G2 molecular set, the binding energies of the weakly bound S22 molecular set, and hydrogen-transfer and non-hydrogen-transfer reaction barrier heights (HTBH38/04 and NHTBH38/04 sets). We found that both SOSEX and RSE corrections to cRPA improve upon the notorious tendency of EX+cRPA to underbind. Surprisingly, reaction barrier heights obtained using EX+cRPA based on a KS reference alone are already remarkably accurate. EX+cRPA+SOSEX+RSE lives up to the challenge of providing a comparable level of accuracy for reaction barrier heights and overall gives the most balanced performance, which holds great promise for widespread application in the future.

- [1] A. Grüneis et al., J. Chem. Phys. 131, 154115 (2009).
- [2] J. Paier et al., J. Chem. Phys. 132, 094103 (2010).
- [2] X. Ren et al., Phys. Rev. Lett. 106, 153003 (2011).

# COHSEX+OCA and COHSEX+DMFT for nanoscopic conductors

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In order to obtain a full first-principles description of the correlated electronic structure and transport properties of atomic- and molecular-size devices we combine the so-called Coherent-Hole-Screened-Exchange (COHSEX) approximation [1] with a fully dynamical treatment of the strongly interacting 3d-electrons of transition metal atoms on the level of the One-Crossing-Approximation (OCA) [2] and the Dynamical Mean-Field Theory (DMFT) [3]. This approach improves upon our recently developed LDA+OCA [5,6] and LDA+DMFT [7] methods for nanoscopic devices, as it allows to calculate the screened Coulomb interaction of the strongly interacting 3d-electrons of the transition metal atoms on a first principles basis. The screened Coulomb interaction is then used as the effective interaction in the dynamical treatment of the strongly interacting 3d-electrons with the OCA impurity solver and the DMFT. We demonstrate the validity of the method by calculating the spectra of some experimentally relevant examples like magnetic adatoms on metal surfaces [8,9] where the Kondo effect is observed.

- [1] M. S. Hybertsen and S. G. Louie, Phys. Rev. B 34, 5390 (1986)
- [2] K. Haule et al., Phys. Rev. B 49, 14211 (1994)
- [3] G. Kotliar et al., Rev. Mod. Phys. 78, 865 (2006)
- [5] D. Jacob, K. Haule, and G. Kotliar, Phys. Rev. Lett. 103, 016803 (2009)
- [6] D. Jacob and G. Kotliar, Phys. Rev. B 82, 085423 (2010)
- [7] D. Jacob, K. Haule, and G. Kotliar, Phys. Rev. B 82, 195115 (2010)
- [8] N. Nel et al., Phys. Rev. Lett. 98, 016801 (2007)
- [9] L. Vitali et al., Phys. Rev. Lett. 101, 216802 (2008)

# Hubbard U from the constrained Random Phase Approximation (cRPA) within a full-potential linearized augmented plane wave approach: Trends for 3d and 4d transition metal perovskites

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Determining the Coulomb interactions in real materials presents a serious challenge for first principles approaches. In 2004, a systematic way - called constrained-RPA (cRPA) - of calculating the Hubbard U and Hund's rule J parameters from first-principles has been proposed by Aryasetiawan and coworkers [1]. We have implemented the cRPA method in the framework of the Full Potential Linear Augmented Plane Waves method as implemented in the Wien2k code [2]. Our scheme permits us to calculate the Hubbard interactions in the same basis in which combined LDA+DMFT calculations are performed within the implementation of [3], yielding a fully consistent first-principles scheme. As an application of cRPA, we have calculated Hubbard U's and Hund J's for cubic 3d and 4d transition metal perovskites [4]. In contrast to what is usually assumed, the trend is not necessarily monotonic, depending on the screening strength and the localization of the wave functions. Our work emphasizes the dependence of U and J on the choice of the one-electron part of the Hamiltonian.

- [1] Aryasetiawan, Imada, Georges, Kotliar, Biermann and Liechtenstein, PRB 70, 195104 (2004).
- [2] Blaha, Schwarz, Madsen, Kvasnicka and Luitz, Wien2k, An Augmented Plane Wave+Local Orbitals Program for Calculating Crystal Properties, Tech. Universitt Wien, Austria, (2001)
- [3] Aichhorn, Pourovskii, Vildosola, Ferrero, Parcollet, Miyake, Georges and Biermann, PRB 80, 085101 (2009)
- [4] Vaugier, Jiang and Biermann, in preparation

## Density functional theory for d-electron systems Are there really strong correlations?

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Density functional theory (DFT) has been established as a powerful method for ground-state properties of materials, but its usefulness is sometimes limited by the accuracy of approximate exchange-correlation functionals. It has long been argued that DFT with the local-density approximation (LDA) and its extensions for exchange-correlation (e.g., with generalized gradient corrections and spin polarization) are not suitable for d-electron systems, especially transition-metal oxides, which are viewed as strongly-correlated materials. Methods such as LDA+U and dynamic mean field theory (DMFT) are widely viewed as the methods of choice for such systems. However, the motivation for developing these methods was originally the energy gap problem, which is not a ground state property and which we now know can be treated by the GW scheme, even for transition-metal oxides. A true test of DFT/LDA would be to examine ground-state properties. This talk will review published and still unpublished results that make the case for the suitability of DFT/LDA for ground-state structural, electronic, and magnetic properties of transition-metal oxides, recognizing at the same time that the approach does not always get the right answer because of the approximate exchange-correlation functionals. The rich variety of properties exhibited by transition-metal oxides is not necessarily the result of strong correlations but of the 10-fold degeneracy of d-orbitals, which facilitates spin ordering and a richness of Jahn-Teller-like effects, giving rise to phenomena that entail coupled electronic, structural, and magnetic degrees of freedom. Work supported by DOE grant DE-FG02-09ER46554

# Spin-orbital polarization in paramagnetic transition metal oxides: $\text{Sr}_2\text{IrO}_4$ versus $\text{Sr}_2\text{RhO}_4$

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We discuss the notions of spin-orbital polarisation and ordering, and address their consequences in transition metal oxides. Extending the combined density functional and dynamical mean field theory (DMFT) scheme as implemented in [1] to the case of materials where spin-orbit interactions are important, we investigate the electronic excitations of the paramagnetic phases of  $\text{Sr}_2\text{IrO}_4$  and  $\text{Sr}_2\text{RhO}_4$ . We show that the interplay of spin-orbit interactions and structural distortions suppresses spin-orbital fluctuations to the extent, that the resulting state in  $\text{Sr}_2\text{IrO}_4$  is a paramagnetic spin-orbital ordered Mott insulator. In  $\text{Sr}_2\text{RhO}_4$ , they lead to a reduced effective band degeneracy, but still keep the material in a (spin-orbitally polarized) metallic state.

[1] M. Aichhorn *et al.*, Phys. Rev. B 80, 085101 (2009).

# **Effective Coulomb and multiplet interactions in correlated electron systems: Experimental determinations and importance of non uniform polarizability.**

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I will discuss the use of model Hamiltonians to describe the electronic structure and elementary excitations in correlated electron systems and the effective parameters that enter into these models. The effective interactions are based on the renormalization of bare interactions resulting from those interactions which are not specifically included in the model. The effective interactions therefore depend critically on which interactions are taken into account explicitly. Also once effective parameters are used the quasi particle weights and single particle spectral functions resulting from the model no longer include the dressing (which is assumed to instantaneously follow the particle) due to these further neglected interactions and their contributions to the coherent and incoherent spectral weights. I will discuss some early fairly direct measurements of the local interactions as obtained from an analysis of the Auger spectra of closed d shell transition metal systems using the multiorbital hubbard model and a two particle greens function approach. These could be regarded as good test cases for ab initio calculations of the interactions. I will also discuss the importance of including the non uniform polarizability in the discussion of the effective parameters. Simple model calculations demonstrate the rather unconventional modifications of the Coulomb interactions in a medium with non uniform polarizability.

# Dynamical screening in correlated electron materials

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The correct notion of the "Hubbard U" in correlated materials is a frequency dependent object which ranges from the (partially) screened static Coulomb interaction of a few eV to the bare Coulomb interaction of about 20 eV at high frequencies. This frequency dependence has not been taken into account in previous ab-initio simulations of materials. I will discuss an efficient method for treating frequency dependent interactions in dynamical mean field calculations, and illustrate the surprisingly large quantitative effects with model calculations and with applications to BaFe<sub>2</sub>As<sub>2</sub>.

# Satellites and large doping- and temperature-dependence of electronic properties in hole-doped $\text{BaFe}_2\text{As}_2$

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Over the last years, superconductivity has been discovered in several families of iron-based compounds. Despite intense research, even basic electronic properties of these materials, such as Fermi surfaces, effective electron masses, or orbital characters are still subject to debate. Here, we address an issue that has not been considered before, namely the consequences of dynamical screening of the Coulomb interactions among Fe-d electrons. We demonstrate its importance not only for correlation satellites seen in photoemission spectroscopy, but also for the low-energy electronic structure. From our analysis of the normal phase of  $\text{BaFe}_2\text{As}_2$  emerges the picture of a strongly correlated compound with strongly doping- and temperature-dependent properties. In the hole overdoped regime, an incoherent metal is found, while Fermi-liquid behavior is recovered in the undoped compound. At optimal doping, the self-energy exhibits an unusual square-root energy dependence which leads to strong band renormalization near the Fermi level.

# Dynamical Vertex Approximation for Nanoscopic Systems

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With the aim of calculating strongly correlated materials more and more reliably, different novel approaches have been proposed in recent years. Quantum Cluster Theories turned out to be very successful for 2- and 3- dimensional Hubbard and related models. Complementary approaches, like Dual Fermion and Dynamical Vertex Approximation, classifiable as diagrammatic extensions of single-site Dynamical Mean Field Theory, become superior when long-range spatial correlations need to be accurately described. An interesting application of Dynamical Vertex Approximation is the one for nanoscopic systems [Phys. Rev. Lett. 104, 246402 (2010)]. The increasing complexity of nanoscopic systems and the possibility of tuning their physical properties through nano-engineering constitutes a new challenge for theories, in particular when strong electronic correlations are involved. I will discuss how Dynamical Vertex Approximation can be applied to such problems. I will show how to model a quantum point contact with 110 atoms and present our finding that the contact becomes insulating already before entering the tunneling regime due to a local Mott-Hubbard transition occurring on the atoms which form the point contact. I will also present results for the realistic case of a manganite nano-cluster where we combined our algorithm with a one- electron Hamiltonian calculated within Density Functional Theory.

# Long range order effects in the Mott-Hubbard transition and the variational lattice approach

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We introduce an efficient strategy to treat long ranged correlations in fermionic lattices, the so called variational lattice approach (VLA). The VLA combines the recently developed dual fermion approach for k-dependent problems and the exact diagonalization technique. We present first benchmark results. The phase diagram of the half-filled paramagnetic Mott-Hubbard transition is discussed and results are compared to CDMFT and DCA calculations.

# Spatial Correlations beyond DMFT: the dual fermion approach

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Incorporating the effects of spatial correlations is a current challenge in the calculation of the properties of materials from first principles. The dual fermion approach[1,2], allows to study spatial correlations beyond dynamical mean-field theory. This contribution illustrates the approach and discusses recent technical advancements, namely, an orthogonal polynomial representation of imaginary time Green's functions[3] and improved estimators for the self-energy and vertex function in the underlying hybridization expansion continuous-time quantum impurity solver[4]. Multiorbital dual fermion calculations are shown to be feasible. In combination with input from bandstructure calculations this facilitates the ab-initio simulation of materials which capture the effects of spatial correlations.

- [1] Hartmut Hafermann, Gang Li, Alexey N. Rubtsov, Mikhail I. Katsnelson, Alexander I. Lichtenstein and Hartmut Monien, *Phys. Rev. Lett.* **102**, 206401 (2009).
- [2] Alexey N. Rubtsov, Mikhail I. Katsnelson and Alexander I. Lichtenstein, *Phys. Rev. B* **77**, 033101 (2008).
- [3] Lewin Boehnke, Hartmut Hafermann, Michel Ferrero, Frank Lechermann and Olivier Parcollet, arXiv:1104.3854, *Phys. Rev. B* **84**, 075145 (2011).
- [4] Hartmut Hafermann, Kelly R. Patton and Philipp Werner, arXiv:1108.1936.

# ***Ab-initio* Calculation of the Magnetic Anisotropy in Transition-Metal Oxides**

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Possible applications in catalysis, spintronics but also as benchmark materials for new experimental techniques such as magnetic exchange force microscopy bring the 3d-transition metal oxides MnO, FeO, CoO, and NiO recurrently into the focus of both experimental as well as theoretical studies. Even though their probably most remarkable property, the existence of an antiferromagnetically ordered ground state at low temperatures, has been studied extensively for years, both the easy axis along which the local magnetic moments align and the magnitude of the magnetic anisotropy are still under discussion. While the magnetic anisotropy in MnO and NiO is expected to originate solely from dipole-dipole interactions, a non-vanishing orbital moment is present in both FeO and CoO and, thus, the anisotropy originating from spin-orbit coupling is believed to be dominant.

We present an *ab-initio* study of electronic and magnetic properties of the 3d-transition metal oxides within density functional theory (DFT) including spin-orbit interaction. To correct for the improper treatment of the on-site Coulomb interaction between the 3d states of the transition metal atoms by (semi-)local density functionals we apply the DFT+ $U$  correction according to Liechtenstein et al.

# ***GW*+EDMFT scheme for a U-V Hubbard model on a two-dimensional square lattice**

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We study a *GW*+EDMFT scheme for the Hubbard model with on-site and nearest-neighbors interactions on a two-dimensional square lattice. Using a continuous-time quantum Monte-Carlo hybridization expansion solver for the solution of the impurity problem, we show how the convergence of EDMFT is affected by the *GW* non-local contributions to the self-energy and polarization, and how this modifies the U-V phase diagram and the spatial properties of the spectral function, for different levels of self-consistency.

# Constructing realistic low energy Hamiltonians for strongly correlated materials from first principles

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The theoretical description of strongly correlated materials is often based on the notion that the main characteristics of these systems can be described by few correlated states localized on certain atoms (e.g. the “ $d$ -states” of the transition metal cation in a transition metal oxide). Similarly, methods such as LSDA+ $U$  and LDA+DMFT generally assume that in many materials of interest, a realistic description of electronic properties can be achieved by an accurate treatment of correlation effects within a small subset of orbitals. The construction of this “correlated subspace”, or more generally of accurate tight-binding (TB) parameterizations for specific subsets of bands, based on first principles electronic structure calculations is therefore an important tool for the study of strongly correlated materials.

Here, we discuss the use of maximally localized Wannier functions to represent the correlated states in different strongly correlated electron materials, and we analyze the differences and uncertainties that result from different choices made in the definition of these “correlated bands”. In particular, we discuss the important case of LaMnO<sub>3</sub>, the parent material for the colossal magneto-resistive manganites [1,2], and the interesting case of rubidium superoxide, RbO<sub>2</sub>, a  $p$ -electron Mott insulator [3].

For LaMnO<sub>3</sub> we compare a parameterization of the electronic structure based on both Mn( $d$ ) and O( $p$ ) states with an “effective  $e_g$ ” picture that involves only two  $e_g$ -like Wannier states per Mn cation. We analyze the effect of both Jahn-Teller and GdFeO<sub>3</sub> distortions on the electronic structure, and compare the TB parameterization obtained from the GGA electronic structure with corresponding parameterizations obtained from GGA+ $U$  calculations with different values for  $U$ .

For the case of RbO<sub>2</sub>, which contains O<sub>2</sub><sup>-</sup> superoxide anions with partially occupied  $p$  states, we demonstrate that this system is indeed a Mott insulator at ambient conditions, but exhibits a strong tendency for orbital ordering at lower temperature, leading to strong coupling between structural, orbital, and magnetic degrees of freedom very similar to the manganite system.

[1] R. Kováčik and C. Ederer, Phys. Rev. B 81, 245108 (2010).

[2] R. Kováčik and C. Ederer, arXiv: 1104.1292 (2011).

[3] R. Kováčik and C. Ederer, Phys. Rev. B 80, 140411 (2009).

# Critical properties of the finite temperature Mott transition in Dynamical Mean Field Theory

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We study the finite temperature Mott transition of the half-filled paramagnetic Hubbard model on the Bethe lattice with infinite connectivity, where Dynamical Mean Field Theory (DMFT) is an exact theory.

The coupled DMFT equations are formulated in terms of a fixpoint problem and solved with a phase space extension approach. The fixpoint surface is analyzed using dynamical systems methods and in particular the Jacobian of the fixpoint function is calculated. The eigenspectra of the Jacobian reveal why the standard forward recursion method is unable to locate all fixpoints in the hysteresis region.

Applying the phase space extension method the hysteresis boundaries and the second order critical end point of the Mott transition line are studied in great detail. The critical end point is shown to be a cusp catastrophe in the parameter space that opens up a pitchfork bifurcation along the first order transition line, while the hysteresis boundaries are saddle-node bifurcations where two fixpoints merge.

Finally the critical properties of the second order end point is analyzed using Landau theory by fitting a minimal Landau model to the fixpoint surface. The excellent agreement between the model and the critical eigen mode of the DMFT fixpoint function leads us to the conclusion that the critical end point have mean field exponents.

For further details see Ref. 1.

- [1] H. U. R. Strand *et. al.*, arXiv:1012.3829v1 [cond-mat.str-el]  
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# Orbital magnetism of late transition metals and actinide monochalcogenides in the LDA+DMFT scheme

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In the last two decades the combination of the density functional theory in local density approximation and the dynamical mean-field theory (LDA+DMFT) has become the standard computational scheme for studying the electronic structure of strongly correlated materials [1]. In this project we use our implementation of the LDA+DMFT scheme into a Full-Potential Linear Muffin-Tin Orbital method (FP-LMTO) [2] to study the orbital magnetism of the itinerant ferromagnets Fe, Co and Ni. In particular the role of the “solver” of the effective impurity problem in the LDA+DMFT scheme is analyzed: the applicability of the spin-polarized T-matrix fluctuation-exchange (SPTF) solver [3] with bare and full propagators is discussed, especially in relation to previous LDA+DMFT simulations [4] and recent experimental photoemission results [5]. A comparison between SPTF and numerically exact Quantum Monte-Carlo method for the corresponding correlation regime is also presented, although limited to models and to a simplified matrix for the Coulomb interaction. Finally our analysis of the orbital magnetism is extended to the actinide monochalcogenides, whose theoretical description still represents a difficult challenge [3].

[1] K. Held, *Advances in Physics* **56**, 829 (2007).

[2] I. Di Marco, *Ph.D. thesis*, Radboud University Nijmegen, 2009

[3] L. V. Pourovskii, M. I. Katsnelson, and A. I. Lichtenstein, *Phys. Rev. B*, **72**, 115106 (2005)

[4] S. Chadov, J. Minár, M. I. Katsnelson, H. Ebert, D. Ködderitzsch, and A. I. Lichtenstein, *Europhysics Letters* **82**, 37001 (2008)

[5] J. Sánchez-Barriga, J. Fink, V. Boni, I. Di Marco, J. Braun, J. Minár, A. Varykhalov, O. Rader, H. A. Dürr, V. Bellini, F. Manghi, H. Ebert, A. I. Lichtenstein, M. I. Katsnelson, O. Eriksson and W. Eberhardt, *Phys. Rev. Lett.* **103**, 267203 (2009)

# An implementation of a CT-QMC solver in the self-consistent LDA-DMFT

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The Density Functional Theory [1, 2] fails to predict accurately both ground state and excited states properties of strongly correlated systems. To correct this, a Hubbard like correction [3] can be added to describe the interaction between correlated electrons. This new formalism can then be solved by the combinaison of the local density approximation (LDA) and the dynamical mean field theory (DMFT) [4] which includes the fluctuations of the interacting electrons. In the DMFT approach, the solution is obtained mapping a lattice model (e. g. Hubbards model) onto a quantum impurity model (e. g. the single impurity model) and imposing a self-consistency condition. The main purpose of this work is to study a new faster solver for the impurity model [5, 6], then to benchmark and compare it to an older solver like the Hirsch-Fye algorithm [7]. Even though these two solvers are quantum Monte Carlo methods, their schemes completely differ. Moreover, although both algorithms can massively run on parallel computers, the continuous-time is more flexible and should be much faster for the species and the temperature range of our interest. The new implementation of this CT-QMC is then apply to transition metals with several 3d or 4f electrons.

- [1] Hohenberg, P. and Kohn, W. Phys. Rev. 136(3B), B864-B871 Nov (1964).
- [2] Kohn, W. and Sham, L. J. Phys. Rev. 140(4A), A1133-A1138 Nov (1965).
- [3] Anisimov, V. I., Zaanen, J., and Andersen, O. K. Phys. Rev. B 44(3), 943-954 ul (1991).
- [4] Georges, A., Kotliar, G., Krauth, W., and Rozenberg, M. J. Rev. Mod. Phys. 8(1) 13 Jan (1996).
- [5] Werner, P., Comanac, A., de' Medici, L., Troyer, M., and Millis, A. J. Phys. ev. Lett. 97(7), 076405 Aug (2006).
- [6] Werner, P. and Millis, A. J. Phys. Rev. B 74(15), 155107 Oct (2006).
- [7] Hirsch, J. E. and Fye, R. M. Phys. Rev. Lett. 56(23), 2521-2524 Jun (1986).

# Dynamical mean field modeling of $\text{LaCoO}_3$

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The interest in  $\text{LaCoO}_3$  arises from its complex magnetic and transport properties [1]. The low-temperature  $\text{LaCoO}_3$  is a non-magnetic insulator. Above 100 K it transforms into a paramagnetic insulator and the metal-insulator crossover takes place around 500 K. The ionic state of Co in this compound is  $\text{Co}^{3+}$ . The 3d orbitals, split to lower three  $t_{2g}$  and upper two  $e_g$ , accommodate six electrons. Depending on the number of  $e_g$  electrons we distinguish the low-spin (LS) state  $t_{2g}^6 e_g^0$  with a spin number  $S = 0$ , the intermediate spin state (IS,  $t_{2g}^5 e_g^1$ ,  $S = 1$ ), and the high spin state (HS,  $t_{2g}^4 e_g^2$ ,  $S = 2$ ). Presently, there are no doubts about prevailing LS character of the low-temperature non-magnetic insulator and the HS character of the paramagnetic metal. Two probable scenarios for the paramagnetic insulator are the LS+HS statistical mixture [2] or the IS [3]. The possibility of the short-range orbitally ordered state with alternating LS+HS and LS sites has also been proposed [4].

We studied the properties of  $\text{LaCoO}_3$  with a dynamical mean field theory (DMFT) combined with local density approximation for non-correlated part [5]. We successfully reproduced the metal-insulator transition. The magnetic crossover cannot be modeled as the temperature is too low for employed DMFT expansion, but we were able to stabilize both non-magnetic and paramagnetic state adjusting the exchange interaction parameter  $J$ . Our results testify to LS+HS scenario of paramagnetic insulator, but we also observed strong hybridization with oxygen p-orbitals, which increases the mean number of electrons on Co atoms to around 6.7 in the non-magnetic and around 6.4 in the paramagnetic state.

- [1] R. R. Heikes, R. C. Miller, and R. Mazelsky, *Physica* **30**, 1600 (1964).
- [2] P. M. Raccach and J. B. Goodenough, *Phys. Rev.* **155**, 932 (1967).
- [3] M. A. Korotin *et al.*, *Phys. Rev. B* **54**, 5309 (1996).
- [4] R. A. Bari and J. Sivardière, *Phys. Rev. B* **5**, 4461 (1972).
- [5] A. Georges *et al.*, *Rev. Mod. Phys.* **68**, 13 (1996).

# A New Analytic Continuation Algorithm for Monte Carlo Data

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A new algorithm for analytic continuation of noisy quantum Monte Carlo (QMC) data from the Matsubara domain to real frequencies is proposed. Unlike the widely used maximum-entropy (MaxEnt) procedure, our method is linear with respect to input data and can therefore be applied to off-diagonal components of a thermal Green's function, or to a self-energy function. The latter possibility is used to analyze QMC results for the half-filled single-band Hubbard model on a Bethe lattice at a low temperature. Our method qualitatively resolves peaks near the inner edges of the Hubbard bands in the vicinity of a Mott transition, whereas a MaxEnt procedure does not. The existence of such structures has been established before in a high-precision D-DMRG calculation by Karski et al (PRB 72, 113110).

# Phase transitions within the GW approximation

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The central concept of the single-band Hubbard model is the competition for the electrons between the tendency to localize for the on-site effective Coulomb repulsion  $U$  and the opposite tendency to hybridize and spread over other lattice sites, which gives rise to a finite bandwidth  $W$ . By varying the  $U/W$  ratio it is possible to obtain a transition from localized to itinerant electronic states. The realisation of this concept can be found in correlated electron materials, where by applying pressure it is possible to induce a transition from an antiferromagnetic insulating to a paramagnetic metallic phase. Here we will discuss metal-insulator transitions in prototypical real systems (e.g. MnO or NiS<sub>2</sub>) using the parameter-free GW approximation of many-body perturbation theory [1]. We will show that the GW approximation is a very useful tool to understand the effects of electronic correlations across the phase transition.

[1] L. Hedin, Phys. Rev. **139**, A796 (1965).

# Optical properties of correlated materials: vanadium dioxide

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The key quantity to describe photoemission spectroscopy is the one-particle Green's function  $G$ . In absorption spectroscopy, instead, one needs to calculate two-particle excitations, which can be obtained from the two-particle correlation function  $L$ . When vertex corrections are neglected (as also usually done in the framework of dynamical mean-field theory [1]),  $L$  can be obtained as a product of two one-particle Green's functions:  $L = -iGG$ . The inclusion of vertex corrections is possible thanks to the solution of the Bethe-Salpeter equation (BSE) [2]. Here we consider a prototypical correlated material, vanadium dioxide ( $\text{VO}_2$ ) in its insulating phase, for which we use a parameter-free BSE approach on top of a self-consistent COHSEX+ $G_0W_0$  calculation of  $G$  [3]. We show that the inclusion of vertex corrections is essential to describe the optical properties of  $\text{VO}_2$ . In particular, we underline the role of crystal local-field effects, associated to the peculiar one-dimensional V-dimer chains, and the effect of excitonic interactions on the absorption onset.

[1] D. N. Basov, R. D. Averitt, D. van der Marel, M. Dressel, and K. Haule, Rev. Mod. Phys. (accepted).

[2] G. Onida, L. Reining, and A. Rubio, Rev. Mod. Phys. **74**, 601 (2002).

[3] M. Gatti, F. Bruneval, V. Olevano, and L. Reining, Phys. Rev. Lett. **99**, 266402 (2007).

# Satellites in Photoemission Spectroscopy

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The  $GW$  method [1] from Many-Body Perturbation Theory (MBPT) has shown to be very successful in the description of photoemission spectra in a variety of systems. In particular,  $GW$  is known to give good quasiparticle properties like band-gaps. However, it has shown some limitations regarding the description of other more complex spectral features like satellites.

Satellite peaks in photoemission come from higher-order excitations, e.g. plasmons, and are still poorly studied in real materials. In one-shot  $GW$  the spectral function  $A(\omega)$  can describe additional features beside the quasiparticle peaks, but these satellites are known to be too weak and too low in energy, as it appears from calculations on the Homogeneous Electron Gas [2] and some real materials [3]. It is not clear whether self-consistency could improve the results. We have thoroughly studied the one-shot  $GW$  spectral function of bulk Si as a test case, trying to understand the flaws of  $GW$  in this respect. Here we compare the theory with new XPS experimental data. These data clearly show multiple plasmon replicas in the photoemission spectrum which are not reproducible within  $GW$ .

The cumulant expansion approximation (CE) for the Green's function, very popular in core-level spectroscopies, has been able to describe satellites correctly within this framework. In the case of valence spectroscopy much less data are available and results are not conclusive [3]. We obtain the cumulant expansion by means of approximations on the 1-particle Green's function's equation of motion, giving a rigorous derivation for this approximation. We show that the CE gives excellent agreement with experiment and discuss how to improve this result even further.

- [1] Hedin, L., Phys. Rev. 139 (1965) A796.
- [2] Hedin, L., Lundqvist, B.I. and Lundqvist, S., J. Res. Natl. Bur. Stand. Sect. A 74A, 417 (1970)
- [3] Aryasetiawan, F., Hedin, L. and Karlsson, K., Phys. Rev. Lett. 77 (1996) 2268; Kheifets, A.S., Sashin, V.A., Vos, M., Weigold, E. and Aryasetiawan, F., Phys. Rev. B 68 (2003) 233205

# Strongly correlated perovskites using local PBE0

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The goal of water photolysis is to split water using only sunlight as the energy input. Complex and in some respect contradicting requirements to the bandstructure have to be fulfilled to avoid photo-corrosion and to achieve maximum light harvesting and maximum conversion efficiency. Because of their complex band structure do perovskite oxides represent particularly interesting candidates for new photo-catalyst materials.[1]

For the description of strongly correlated oxides, either local model theories, such as LDA+U or LDA+DMFT, or expensive non-local hybrid functionals, with a portion of exact exchange, are being used. A local formulation of the *PBE0* hybrid functional is, therefore, implemented into the CP-PAW Code, which also provides a link to LDA+U. The description of the local subspace is inspired by the LMTO framework, energy independent and applicable to multiple shells. Moreover, the contribution from the core is taken into account.[2]

The method is applied to various perovskite oxides.

- [1] Ch. Jooss, D. Mierwald, J. Hoffmann, M. Uijtewaal and P. Blöchl, *Perovskite oxides for photoinduced water splitting*, to be published.
- [2] M.A. Uijtewaal, C.F.J. Walther and P.E. Blöchl, *PBE0 implemented into PAW with energy independent localized orbitals*, to be published.

# LDA+DMFT(ED) study of Transition Metal Monoxides

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The electronic structure of the late transition monoxides – MnO, FeO, CoO, and NiO – is addressed using Exact Diagonalization within the LDA+DMFT scheme. The interplay between the strong correlation of the localized 3d-states of the transition metal, and the strong hybridization with the itinerant oxygen 2p-states, pose a major theoretical and technical challenge. Through the use of sets of conserved quantum numbers, the finite temperature calculations are performed with up to 20 auxiliary spin orbitals in the impurity solver, and allowed to reach full charge self-consistency in the LDA+DMFT scheme. The calculated spectra approach the experimental photoemission spectra as more auxiliary states are added, but a full convergence in the number of auxiliary states is currently prohibitively expensive in terms of computational resources. Other technical challenges, like the effect of an incomplete basis on the hybridization function, and possible solutions to these challenges, are highlighted in the poster.

# Dichotomy between Large Local and Small Ordered Magnetic Moments in Iron-Based Superconductors

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We study a four-band model for iron-based superconductors within the local density approximation combined with dynamical mean-field theory (LDA+DMFT)[1]. This successfully reproduces the results of models which take As p degrees of freedom explicitly into account and has several physical advantages over the standard five d-band model. Our findings reveal that the new superconductors are more strongly correlated than their single-particle properties suggest. Two-particle correlation functions unveil the dichotomy between local and ordered magnetic moments in these systems, calling for further experiments to better resolve the short time scale spin dynamics.

- [1] P. Hansmann, R. Arita, A. Toschi, G. Sangiovanni, K, Held, Phys. Rev. Lett. **104**, 197002 (2010)

# Hyperfine field and local spin magnetic moment of $\text{Fe}_{3-x}\text{Mn}_x\text{Ge}$ Heusler alloys: DFT study

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Density functional theory based on full potential linearized augmented plane wave (FP-LAPW) method is used to investigate the hyperfine field and local magnetic moment at different atomic sites in  $\text{Fe}_{3-x}\text{Mn}_x\text{Ge}$  Heusler alloys, where ( $0 \leq x \leq 3$ ). Alloys with  $x < 2$  are found to exhibit a ferromagnetic phase, whereas the rest have shown ferrimagnetic phase. The calculated local spin magnetic moments of Mn[B] sites roughly stay concentration independent for different alloys ( $\sim 2.65 \mu_B$ ), while the Fe[A,C] and Mn[A,C] site moments increase with  $x$ . Also, the magnetic hyperfine field of Ge atoms increase with increasing Mn concentration, it is varying from 69.3 KG at  $x=0$  to 373.9 KG at  $x=3$ . Our calculated values for the spin magnetic moment and hyperfine fields closely agree with the previous experimental results.

- [1] S. Ishida, S. Asano and J. Ishida, J. Phys. Soc. Jpn. 53 (1984) 2718.
- [2] S. Sarkar and C. Bansal, J. Alloys and Compounds 366 (2004) 107.

# A unified description of ground and excited state properties of finite systems: the self-consistent $GW$ approach

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Fully self-consistent  $GW$  (sc- $GW$ ) – based on the iterative solution of Dyson’s equation – incorporates many-body correlation effects in the electronic ground-state, providing a recipe to consistently describe ground- and excited-states on an equal footing. We have implemented sc- $GW$  in the localized basis all-electron code FHI-aims [1]. We show that, for finite systems, the ground-state properties as well as the excitation spectrum of the sc- $GW$  Green’s function are unique and are not affected by different initialization of the sc- $GW$  loop, curing the pathological dependence on the starting point of one-shot  $GW$  ( $G_0W_0$ ). In addition, self-consistency systematically improves ionization energies and Galitskii-Migdal total energies of closed shell systems compared to  $G_0W_0$  based on Hartree-Fock and density-functional theory in local and semilocal approximations. Moreover, our implementation is based on interacting Green’s functions – unlike all  $G_0W_0$  implementations – hence it moves a first step towards going beyond the  $GW$  approach.

[1] V. Blum *et al.*, *Comp. Phys. Comm.* **180**, 2175 (2009).

# Unravelling the $\alpha$ - $\gamma$ phase transition in Ce from the nanoscale to bulk

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The first-principles description of  $f$ -electron systems is currently regarded as one of the great challenges in condensed matter physics. The simultaneous presence of itinerant  $spd$ -states and localized partially occupied  $f$ -states and their mutual interaction in rare-earth materials gives rise to a rich variety of physical phenomena that continue to be a testing ground for electronic structure theories. Cerium, for example, undergoes an iso-structural  $\alpha$ - $\gamma$  phase transition that is accompanied by a large volume collapse of 15% at room temperature and ambient pressure.

In this work we apply the cluster extrapolation approach [1] to the problem of the  $\alpha$ - $\gamma$  phase transition. The electronic structure of each cluster is determined using hybrid density functionals (e.g. PBE0) and full exact-exchange plus correlation at the level of the random phase approximation (EX+cRPA).

For all clusters we find, at the PBE0 level, two stable configurations with different lattice constants and distinct electronic and magnetic properties, indicative of the phase transition in bulk Ce. While hybrid functionals incorrectly predict the high volume phase (linked to the  $\gamma$  phase) to be most stable at zero temperature, the correct energetic ordering is recovered in EX+cRPA where exact-exchange is screened in a physically meaningful way. This happens in correspondence with a higher density of states at the Fermi level for the  $\alpha$ -phase-like solution, in agreement with photoemission experiments [2]. Our zero-temperature results show a change in the degree of localization of the  $f$ -states and complement previous LDA+DMFT studies (which for technical reasons are restricted to the high-temperature regime), indicating that a first principles description of Ce within the framework of DFT is possible.

- [1] Qing-Miao Hu, Karsten Reuter, and Matthias Scheffler, *Phys. Rev. Lett.* **98**, 1 (2007).  
[2] M. Grioni *et al.*, *Phys. Rev. B* **55**, 2056 (1997).

# Charge Kondo theory of PbTe doped with Tl impurities

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Semiconducting PbTe is one of the most interesting materials for thermoelectric applications. When doped with a small concentration of Tl impurities, acting as acceptors, a number of anomalous properties are found: e.g., beyond a critical concentration of about 0.3 at.% Tl, the system exhibits superconductivity with remarkably high critical temperatures for such a low carrier system. This and other anomalous phenomena prompted the idea that Tl impurities act as negative U centres leading to a charge Kondo effect [1] and to superconductivity. In this talk, we combine ab-initio information [2] and numerical renormalization group methods to explore the consequences of this model for the normal state properties, showing that it can explain a number of features in the temperature and doping dependence of the resistivity, carrier density and thermopower [3].

[1] S. Andergassen, T. A. Costi and V. Zlatić, arXiv:1101.4124.

[2] D. J. Singh, Phys. Rev. B **81**, 195217 (2010).

[3] T. A. Costi and V. Zlatić, preprint.

# A simple DFT-based perspective on correlated materials

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For all its successes in predicting materials properties from first principles, density functional theory in its common flavors (LDA, GGA) tends to fail, sometimes qualitatively, for correlated materials. Of the many shortcomings (locality, static screening, etc.) of the DFT exchange-correlation potential (i.e. DFT's own approximate self-energy), its built-in self-interaction is particularly severe.

In recent years, our group has been applying and further developing a simple and inexpensive self-interaction correction approach originally proposed by Filippetti and Spaldin. This scheme cures some outstanding failures of standard DFT for correlated systems while retaining a realistic level of materials description (see a review in [1]). In particular, it provides gaps and magnetism for Mott-like systems such as cuprates, titanates, and manganites: this is a key stepping stone for further studies, which are instead precluded to LDA, or GGA, which find Mott-like insulators to be metallic and non magnetic. Recently, we also obtained a variational formulation of the method and an expression of quantum forces.

Beside discussing the method, I will review a selection of the numerous recent applications, such as multiferroic manganites (e.g.  $\text{Pr}_{0.5}\text{Ca}_{0.5}\text{MnO}_3$  [2]), low-dimensional cuprates (e.g. polaronic 1D Ca-doped  $\text{YCuO}$  [3]), insulator-insulator metallic interfaces [4], and small-gap d1 titanates [5].

This work stems from a long-standing collaboration with A. Filippetti, with contributions by P. Delugas, G. Colizzi, D. Puggioni, G. M. Lopez, and G. Peralta.

- [1] A. Filippetti and V. Fiorentini, *Eur. Phys. J. B* 81, 139 (2009).
- [2] G. Colizzi, A. Filippetti, and V. Fiorentini, *Phys. Rev. B* 82, 140101(R) (2010)
- [3] A. Filippetti and V. Fiorentini, *Phys. Rev. B* 77, 235124 (2008).
- [4] P. Delugas et al., *Phys. Rev. Lett.* 106, 166807 (2011).
- [5] A. Filippetti et al., to be published.

# Electronic correlation and many body effect: studies on some paradigmatic metal oxides

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Correlation gives rise to spectacular observations in experiment, such as superconductivity, or the fractional Quantum Hall effect. At the same time, it is very difficult to treat correlation from the theoretical point of view: today, although the underlying interaction (the Coulomb interaction) is simple and well understood, a unifying ab initio framework that would allow us to describe, analyze, understand and predict all those correlation-related phenomena on the same footing is still missing. In this work we will illustrate some electronic and optical properties of metal oxides systems, like vanadium sesquioxides ( $V_2O_3$ ,  $V_2O_5$ ) or perovskites like  $LaTiO_3$  or  $YTiO_3$ , where electronic correlation is treated through a complete ab initio Green's Function Many Body Perturbation Theory framework

# Spectral and optical properties of Mott antiferromagnets

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We address the problem of optical conductivity in Mott antiferromagnets. In particular we perform model dynamical mean field theory calculations, using Bethe lattice, for Hubbard model in the long range order antiferromagnetic phase. Further insight is gained by using both a numerically exact method and a (computationally cheaper) approximated method, which exploits the mapping onto the  $t - J$  model. This allows us to determine the characteristic shape of the optical conductivity of a Mott antiferromagnet. Our study is motivated by the interesting experimental observation of multiple peaks in the optical conductivity of Mn-based compounds whose origin has not yet been understood, and allows us to obtain a possible benchmark for the presence of antiferromagnetism arising from strong correlations.

# Dynamics of Electronic States at the Surface of Bismut

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Time-resolved photoemission experiments now o more possibilities of exploring the out-of-equilibrium electronic structure of materials. The Femto-ARPES group has newly been established in Synchrotron SOLEIL (Saint-Aubin, France) under the guidance of Professor Luca Perfetti and has been working recently on photoinduced transitions and photo-excitations, in compounds such as vanadium dioxyde or charge-density-wave materials. We present the results of our investigations on Bismuth(111). Time-resolved ARPES measurements reveal momentum-localized energy oscillations of bulk-derived states. The mechanism of this observation is discussed, and linked to the photo-generation of coherent phonons in Bismuth. We thus measure the electron-phonon coupling parameter.

