Vienna Computational Materials Laboratory

ViCoM

ViCoM Workshop April 2012

(12.04.2012-13.04.2012)

Programme & Schedule

Programme

Project Part o2 “Towards Exact Correlation in Extended Systems”

Principal Investigator/ Project Part Leader: Georg Kresse

Project Part	Date & Time	Presentation by
P02 Towards Exact Correlation in Extended Systems	12.04., 10:20 – 10:50	**Andreas Grüneis**
	Wavefunction based treatment of electronic correlation in solids Wavefunction based methods such as second-order Moller-Plesset perturbation, coupled-cluster and full Configuration Interaction (CI) theory form a hierarchy of increasingly accurate methods that is well established in the field of computational quantum chemistry. We seek to apply this range of methods to the problem of electronic correlation in solid state systems. We have implemented the second-order Moller-Plesset perturbation theory (MP2) and coupled-cluster methods (CCSD and CCSD(T)) within the framework of the full-potential Projector-Augmented-Wave (PAW) method, using periodic boundary conditions and a plane wave basis set in VASP.[1,2,3] Moreover, an interface between VASP and the Full CI quantum Monte Carlo (FCIQMC) code presented in Ref.[4] was developed. However, the computational cost of the above methods quickly becomes intractable with increasing system size. We outline techniques that reduce the computational effort significantly such as the use of explicitly correlated wavefunctions. Moreover we present results for archetypal solid state systems that were calculated using the above methods. [1] M. Marsman, A. GrÃŒneis, J. Paier, and G. Kresse, J. Chem. Phys. 130, 184103 (2009). [2] A. GrÃŒneis, M. Marsman, and G. Kresse, J. Chem. Phys. 133, 074107 (2010). [3] A. GrÃŒneis, G. H. Booth, M. Marsman, J. Spencer, A. Alavi, and G. Kresse, J. Chem. Theory Comput., 7, 2780 (2011). [4] G. H. Booth, A. J. W. Thom, and A. Alavi, J. Chem. Phys. 131, 054106 (2009).	

Project Part 03 “Dynamical Mean Field Theory and Beyond”

Principal Investigator/ Project Part Leader: Karsten Held

Research Partner / National Partner: Enrico Arrigoni

Project Part	Date & Time	Presentation by
PO3 / A Dynamical Mean Field Theory and Beyond	12.04., 10:50 – 11:00	**Karsten Held**
	Project and cooperation overview	

Project Part 03 “Dynamical Mean Field Theory and Beyond”

Principal Investigator/ Project Part Leader: Karsten Held

Research Partner / National Partner: Enrico Arrigoni

Project Part	Date & Time	Presentation by
PO3 / B Dynamical Mean Field Theory and Beyond	12.04., 11:00 – 11:25	**Ciro Taranto**
	Merging GW and dynamical mean-field theory The combined approach of local density approximation (LDA) and dynamical mean-field theory (DMFT) represents the state-of-the-art for the study of strongly correlated materials. Nevertheless the predictive power of this approach is limited by two principal issues: the problem of extimating ab initio the screened Coulomb interaction and to determine unambiguously the so called double-counting corrections. Both problems are rooted in the conceptual diffi culty of formulating the DMFT and the LDA in a common context, since DMFT is usually expressed in terms of Feynman diagrams, while LDA is not. For this reasons we believe that the GW +DMFT [1] approach, which allows also for a diagrammatic formulation [2], can represent a major improvement to the LDA+DMFT one. Specifically, we show how one can interface the GW approach with the DMFT in a possibly self-consistent cycle. To show the feasibility of the proposed method, we also present our preliminary GW +DMFT results on the test-material SrVO3 . [1] S. Biermann, F. Aryasetiawan and A. Georges, Phys. Rev. Lett. 90 086402 (2003). [2] K. Held, C. Taranto, G. Rohringer, A. Toschi, in Proceedings of the LDA+DMFT approach to strongly correlated materials school, J¨ulich, (2011), edited by E. Pavarini, E .Koch, D. Vollhardt and A. Lichtenstein (2011) [arXiv:1109.3972] .	

Project Part o4 “Quantum Impurity Solvers”

Principal Investigator/ Project Part Leader: Frank Verstrate

Research Partner / National Partner: Gerd Evertz

Project Part	Date & Time	Presentation by
P04 Quantum Impurity Solvers	12.04., 14:10 – 14:40	**Martin Nuss**
	“Strongly correlated quantum dot out of equilibrium: A variational cluster approach” The theoretical understanding of the non-equilibrium behavior of strongly correlated quantum many body systems is a long standing challenge, which has become increasingly relevant with the progress made in the fields of molecular- and nano- electronics, spintronics or quantum optics and simulation. We report on the development of non-equilibrium cluster perturbation theory, and its variational improvement, the non-equilibrium variational cluster approach. These non-equilibrium extensions of well-established equilibrium approaches are based on the Keldysh Green's function method which allows, in this case, to access single particle dynamic quantities on the whole complex plane. These flexible and versatile techniques can in principle be applied to any lattice Hamiltonian with local interactions, including multi-band and multi-impurity systems. Within this framework it is possible to work in the thermodynamic limit and therefore exchange particles with a bath and/or dissipate energy. We will highlight the importance of the self-consistently determined variational parameters which are introduced in the non-equilibrium variational cluster approach. We will discuss the performance, open issues and limitations as well as the advantages of the non-equilibrium variational cluster approach on the basis of a single impurity system, for which this method performs well in the equilibrium situation. Results for the steady state current density as well as the non-equilibrium density of states of a strongly correlated single quantum dot will be presented. They will be compared to and benchmarked against data for the time evolution and quasi stationary state obtained using matrix product state based methods.	

Project Part o5 “Embedded Cluster Approach and Non-Adiabatic Processes in Physics and Chemistry”

Principal Investigator/ Project Part Leader: Joachim Burgdörfer

Research Partner / National Partner: Hans Lischka

Project Part	Date & Time	Presentation by
P05 Embedded Cluster Approach and Non-Adiabatic Processes in Physics and Chemistry	12.04., 11:25 – 11:55	**Paul Tiwald**
	“A Proton interacting with a LiF surface: an embedded cluster approach” We apply high-level tools of quantum chemistry such as the multi-configuration self-consistent field (MCSCF) and multi-reference configuration interaction (MRCI) method to describe the interaction of a proton with a LiF surface. In our approach the LiF surface is represented by a small active cluster which is embedded into a surrounding matrix mimicking the infinite crystal. For a model system in which the active cluster consists of a single fluorine ion and five surrounding lithium ions we present first results on the interaction dynamics such as the neutralization probability of a proton scattered off a LiF surface.	

Project Part o6 “Dynamical Correlated Systems”

Principal Investigator/ Project Part Leader: Norbert Mauser

Research Partner / National Partner: Armin Scrinzi

Project Part	Date & Time	Presentation by
P06 Dynamical Correlated Systems	13.04., 10:45 – 11:15	**Armin Scrinzi**
	“Photo-emission, excitation, and fields on surfaces: progress report P06” For the integration of dynamics with structure codes, maximal advantage of the highly developed structure calculations must be taken. As a first example, an interface of the quantum chemical COLUMBUS package to quantum dynamics will be introduced with its application dissociative photoionization. In the interaction of strong fields with surfaces, modifications of the field by the surface must be taken into consideration. Changes of polarization and field enhancement significantly modify the local field. Implications for dynamic measurements and applications for new sources will be discussed. Finally, a newly developed for computing single- and double photo-electron spectra will be introduced and illustrated with examples.	

Project Part o7 Electronic Structure of Solids, Surfaces and Nanostructures

Principal Investigator/ Project Part Leader: Peter Blaha

Project Part	Date & Time	Presentation by
P07 / A Electronic Structure of Solids, Surfaces and Nanostructures	12.04., 13:30 – 13:50	**Hans-Peter Koch**
	"Adsorption of Au atoms on the h-BN/Rh(111) nanomesh" The h-BN/Rh(111) nanomesh [1] consists of a highly corrugated single layer of h-BN on a Rh(111) surface. Due to the lattice mismatch a nanostructure with a periodicity of 3.2 nm is formed. In this nanostructure BN forms ``pores'' of about 2 nm, which are separated by ``wires'', where BN is 0.1 - 0.2 nm further away from the transition metal than in the ``pores''. The ``pores'' of the nanomesh show the extraordinary ability to trap molecules and metallic clusters - forming well-ordered arrays and prohibiting aggregation. We have theoretically studied the adsorption of Au atoms on bulk h-BN and on various models of the h-BN/Rh(111) nanomesh. While Au binds only weakly to bulk h-BN and h-BN/Rh(111) at the ``wire'' configurations, the underlying Rh atoms in the ``pores'' modify considerably the electronic structure of h-BN and Au adsorbs strongly on top of the B atoms. The adsorption is accompanied by a strong outward relaxation of the B atoms and a significantly charging of the Au atoms [2]. Furthermore, we will present first results of the adsorption of small Au[n] clusters (n=2-4) in the ``pores''. Their adsorption properties show similar trends as observed for single Au atoms. [1] M. Corso et al., Science 303: 217 (2004) [2] HP. Koch et al., Phys. Rev. B 84: 245410 (2011)	

Principal Investigator/ Project Part Leader: Peter Blaha

Project Part	Date & Time	Presentation by
P07 / B Electronic Structure of Solids, Surfaces and Nanostructures	12.04., 13:50 – 14:10	**Fabien Tran**
	"Hybrid functionals in WIEN2k: implementation and applications" The screened and unscreened hybrid functionals were recently implemented into the WIEN2k code [1]. Results obtained with the hybrid functionals PBE0 and YS-PBE0 for the calculation of the F center in LiF and the electronic and magnetic properties of CrN will be presented. There will be also a discussion of the various approximations which can be done to make calculations with hybrid functionals faster, e.g., considering only the diagonal elements of the 2nd Hamiltonian [2] or using a reduced k-mesh for the screened Hartree-Fock potential. [1] F. Tran and P. Blaha, Phys. Rev. B 83, 235118 (2011). [2] F. Tran, Phys. Lett. A 376, 879 (2012).	

Project Part 09 “Complex Magnetic Structures”

Principal Investigator/ Project Part Leader: Peter Mohn

Research Partner / National Partner: Josef Redinger

Project Part	Date & Time	Presentation by
P09 / A Electronic Structure of Solids, Surfaces and Nanostructures	12.04., 16:00 – 16:30	**Marcel Hieckel**
	“Ab-initio studies of bulk and surface properties of SrRuO3 and Sr3Ru2O7” Perovskite oxide materials have attracted enormous attention because of a variety of intriguing physical properties. In this context, we present results of density functional theory (DFT) calculations for the bulk materials $SrRuO_3$ and $Sr_3Ru_2O_7$ and the [001] surface of $Sr_3Ru_2O_7$. For the exchange-correlation functional the generalized gradient approximation of Perdew-Burke-Ernzerhof [1] was used and further studies were made with post-DFT concepts such as hybrid functional [2] and GW approaches [3]. Structural, electronic and magnetic properties were investigated for both systems including simulations of scanning tunneling microscopy experiments [4] for a freshly cleaved $Sr_3Ru_2O_7$ [001] surface. Work supported by the FWF SFB FOXSI (F4511-N16), the Doctorate College CMS at the TU Wien and by computer time from the VSC. [1] J. P. Perdew, K. Burke, and M. Ernzerhof, Phys. Rev. Lett. 77, 3865 (1996). [2] A. V. Krukau et al., J. Chem. Phys. 125, 224106 (2006). [3] L. Hedin, Phys. Rev. 139, A796 (1965). [4] J. Tersoff and D. R. Hamann, Phys. Rev. B 31, 805 (1985).	

Project Part o9 “Complex Magnetic Structures”

Principal Investigator/ Project Part Leader: Peter Mohn

Research Partner / National Partner: Josef Redinger

Project Part	Date & Time	Presentation by
P09 / B Electronic Structure of Solids, Surfaces and Nanostructures	12.04., 16:30 – 17:00	**Robert Achleitner**
	Low Temperature broadening of the NMR-Spectra of Spin-Ladder Compounds with small Impurity-Concentration; A QMC Simulation We apply a highly parallelized Quantum Monte Carlo (QMC) code with a directed loop algorithm to the spin ladder structure assumed for SrCu2O3 where single spin ladders are coupled to each other. For these systems we generate the local magnetic moment profiles caused by non magnetic impurities, which are simulated by missing spins (vacancies). In our calculations we analyse the behaviour of single ladders consisting of 200x2 spins up to 8 coupled ladders with a total of 3200 spins with periodic boundary conditions. Our calculations allow for a qualitative description of the experimentally observed broadening of the NMR lines upon reduction of the temperature.	

Project Part 10 “Multi-Scale Simulations of Multi-Component Phases”

Principal Investigator/ Project Part Leader: Raimund Podlouky

Research Partner / National Partner: Jürgen Hafner, Ernst Kozeschnik

Project Part	Date & Time	Presentation by
P 10 Multi-Scale Simulations of Multi-Component Phases	12.04., 13:00 – 13:30	**Tobias Kerscher**
	Monte-Carlo simulations with DFT accuracy: transcending scale and time with the cluster expansion The cluster expansion (CE) is a mighty tool to bridge the gap of scale and time in ab initio based methods. In combination with Monte-Carlo simulations, large-scale systems in the micrometer range and the kinetics of vacancy-mediated diffusion processes become available. We present advances in the CE method as implemented in the Monte-Carlo routines of UNCLE [1]. On the one hand, UNCLE comprises a weak-scaling parallel Monte-Carlo algorithm [2], which is applied on the macroscopic scale to the ternary bulk system of B2 NiAl with one billion atomic sites. On the other hand, we take first steps towards accurate diffusion kinetics with the CE. Our modeling of the diffusion jumps will incorporate many-body effects as well as variable transition barriers that depend on the structural environment of the jump, which is paramount for the calculation of MC jump rates according to transition state theory. [1] D. Lerch et al., Modelling Simul. Mater. Sci. Eng. 17 (2009), 055003 [2] T. C. Kerscher et al., IPDPS 1234 (2011)	

Project Part 11 “Nucleation and Self-Assembly in Soft Matter Systems: From the Molecular to the Mesoscopic Scale”

Principal Investigator/ Project Part Leader: Christoph Dellago

Research Partner / National Partner: Gerhard Kahl

Project Part	Date & Time	Presentation
P11 Nucleation and Self-Assembly in Soft Matter Systems: From the Molecular to the Mesoscopic Scale	12.04., 17:00 – 17:30	**Ulf Pedersen**
	Novel method for computing Gibbs energy of phases In computational studies, first order transitions are easily bypass since they (typically) rely on a rare event of homogeneous nucleation. Thus, it is not feasible to simply change pressure and temperature to determine coexistence lines in the phase diagram. We introduce a novel method for computing Gibbs energy difference between phases -- not relying on nucleation. In short, the strategy is to compute the average force on the interfaces of a two-phase crystal/liquid system. This force depend on the Gibbs energy difference between the phases and is computed by applying an external field coupling to long-range translational order. The method is validated for the crystal/liquid coexistence line of the Lennard-Jones system, and overcome some shortcomings of other Gibbs energy methods found in literature.	

Project Part 12 “Multi-Scale Simulations of Magnetic Nanostructures”

Principal Investigator/ Project Part Leader: Dieter Süss

Research Partner / National Partner: Thomas Schrefl

Project Part	Date & Time	Presentation by
P12 Multi-Scale Simulations of Magnetic Nanostructures	13.04., 9:45 – 10:15	**Lukas Exl**

“Micromagnetic energy minimization for low-rank tensor magnetization “

A tensor grid algorithm for the minimization of the micromagnetic energy is presented. Based on the method of multipliers [1] this approach allows the treatment of the micromagnetic side constraint in a tensor-structured framework [2], but also offers a competitive alternative to well-established approaches in numerical micromagnetics for non-tensor-structured considerations. Since energy components and their gradients can be computed efficiently for low-rank tensor magnetizaton (e.g. Tucker tensors) [3], the algorithm shows sub-linear complexity with respect to the grid size in terms of costs per iteration [4]. Apart from that, the ill-conditioning of the unconstrained subproblems usually arising in penalty-like methods is overcome, which is shown by estimates on the convergence rate. We compare with results of the Standard Problem No.3 posed by the μMAG micromagnetic modeling activity group at the National Institute of Standards and Technology (NIST) [5].

References

[1] D.P. Bertsekas Multiplier Methods: A Survey. Automatica, 12:133–145, 1976.

[2] B.N. Khoromskij Tensor-structured numerical methods in scientific computing: Survey on recent advances. Chemometrics and Intelligent Laboratory Systems, 110:1–19, 2012.

[3] Exl, L. and Auzinger, W. and Bance, S. and Gusenbauer, M. and Reichel, F. and Schrefl, T. Fast stray field computation on tensor grids. Journal of Computational Physics, 231:2840–2850, 2012.

[4] Exl, L. and Schrefl, T. and Mauser, N.J. and Stimming, H.P. Micromagnetic energy minimization for low-rank tensor magnetization. in preparation.

[5] McMichael, R.D. Standard Problem Number 3, Problem Specification and Reported Solutions, Micromagnetic Modeling Activity Group, http://www.ctcms.nist.gov/~rdm/mumag.html, 1998.

Guest Lecture

Project Part	Date & Time	Presentation
Guest Lecuture	13.04., 9:00 – 9:45	**Carsten Honerkamp -** Institute for Theoretical Solid State Physics, RWTH Aachen University
	Getting more specific: the functional renormalization group and materials? In fermionic many-body systems, renormalization group (RG) methods are traditionally used for qualitative statements about the low-energy state or long wave-lengths from which universal information might be obtained. On the other hand, the RG framework is a rather comprehensive approach to the physics at many scales, and hence it should be possible to use RG schemes for the exploration of non-universal, quantitative questions and material trends. Here I will present new applications of the functional RG in the field of iron arsenide superconductivity and in the question of possible interaction-driven ground states in bilayer graphene. I will also briefly discuss functional RG extensions of the constrained-RPA scheme for the computation of low-energy effective interactions.	

Guest Lecture

Project Part	Date & Time	Presentation by
Guest Lecuture	12.04., 14:40 – 15:25	**Andrea Marini -** Istituto di Struttura della Materia (ISM), Consiglio Nazionale delle Ricerche (CNR)
	"Electron-phonon mediated de-phasing in electronic systems driven out-of-equilibrium by ultra-strong laser pulses" Ultra-fast optical spectroscopy is a powerful tool for the observation of dynamical processes in several kind of materials. The basic time-resolved optical experiment is the so-called "pump-probe": a first light pulse, the "pump", resonantly triggers a photo-induced process. The probe pulse photon energy, spectral width and peak intensity creates a certain density of electron-hole pairs in a more or less localized region of space. The subsequent system evolution can be monitored, for example, by the time-dependent transmission changes of a delayed "probe" pulse. After the creation of the initial carrier density the time evolution of the single-particle and many-particle excitations is now governed by a non-trivial interplay between phase coherence and energy relaxation. Indeed, scattering processes tend to destroy the coherence, leading to a de-phasing of the excitations. The role of the electronic correlations at this stage is to stabilize the ensemble by creating quasi-particles and multi-particle states. De-phasing will be driven by different phenomena. One of the most important is the energy transfer to the atomic motion in form of phonon excitations. In this talk I will present a novel approach based on the merging of Non-Equilibrium Green's function theory and Density Functional Theory to treat the phonon-mediated relaxation following the pump excitation. I will discuss key theoretical and methodological aspects of the basic tools, the Kadanoff-Baym equations (KBE), by presenting simulations of the pumped electrons dynamics in paradigmatic materials. In particular I will discuss how the memory dependence naturally embodied in the KBE's can be formally rewritten as an iterative approach that drastically reduces the simulation time.	

Guest Lecture

Project Part	Date & Time	Presentation by
Guest Lecuture	12.04., 9:05 – 9:50	**Andreas Laeuchli** - Institut für Theoretische Physik, Universität Innsbruck
	"The Quest for New Quantum States of Matter: Computational Approaches to Quantum Many Body Systems" The discovery and understanding of new states of quantum matter is of central interest for basic research as well as for potential future technological applications. In this talk we review our recent activity on computer simulation driven discoveries and characterizations of exotic phases in quantum magnetism, correlated electron systems and ultracold atomic gases.	

Schedule

Thurdsday, 12.04.2012			
Time	Title	Presenter/s	Details
9:00 – 9:05	Greetings / Introduction	Georg Kresse	Greetings, Announcements
9:05 – 9:50	"The Quest for New Quantum States of Matter: Computational Approaches to Quantum Many Body Systems"	Andreas Laeuchli	Guest Lecture , 45 min, discussion included (5 min.)
9:50 – 10:20	Coffee Break		
10:20 – 10:50	Wavefunction based treatment of electronic correlation in solids	Andreas Grüneis	P02, 30 min.
10:50 – 11:25	Project and cooperation overview	Karsten Held	P03/A, 10 min.
	"Merging GW and dynamical mean-field theory"	Ciro Taranto	P03/B, 25 min.
11:25 – 11:55	"A Proton interacting with a LiF surface: an embedded cluster approach"	Paul Tiwald	P05, 30 min.
12:00 – 13:00	Lunch		
13:00 – 13:30	"Monte-Carlo simulations with DFT accuracy: transcending scale and time with the cluster expansion"	Tobias Kerscher	P10, 30 min.

13:30 – 14:10	"Adsorption of Au atoms on the h-BN/Rh(111) nanomesh"	Hans Peter Koch	P07/A, 20 min.
	"Hybrid functionals in WIEN2k: implementation and applications"	Fabien Tran	P07/B, 20 min.
14:10 – 14:40	"Strongly correlated quantum dot out of equilibrium: A variational cluster approach"	Martin Nuss	P04, 30 Min.
14:40 – 15:25	"Electron-phonon mediated de-phasing in electronic systems driven out-of-equilibrium by ultra-strong laser pulses"	Andrea Marini	Guest Lecture , 45 min,., discussion included (5 min.)
15:30 – 16:00	Coffee Break		
16:00- 16:30	"Ab-initio studies of bulk and surface properties of SrRuO3 and Sr3Ru2O7"	Marcel Hieckel	P09/A, 30 min.
16:30 – 17:00	"Low Temperature broadening of the NMR-Spectra of Spin-Ladder Compounds with small Impurity-Concentration; A QMC Simulation"	Robert Achleitner	P09/B, 30 min.
17:00 – 17:30	"Novel method for computing Gibbs energy of phases"	Ulf Pedersen	P11, 30 Min
17:30	5. Mitgliederversammlung		
19 Uhr	Dinner, Universitätsbräuhaus		

Friday, 13. 04. 2012			
9:00 – 9:45	"Getting more specific: the functional renormalization group and materials?"	Carsten Honerkamp	Guest Lecture , 45 min,., discussion included (5 min.)
9:45 – 10:15	"Micromagnetic energy minimization for low-rank tensor magnetization "	Lukas Exl	P12, 30 min.
10:15 – 10:45	Coffee Break		
10:45 – 11:15	"Photo-emission, excitation, and fields on surfaces: progress report P06"	Armin Scrinzi	P06, 30 min.
11:15 - 12:00	Discussion		
12:00 – 13:30	Lunch "Culinarium Cooking"		