PROGRAMME

Location	"Baumkircher Konferenzsaal" in the "Burg Schlaining"-Castle, A-7461 Stadtschlaining, Austria

Guest Lecture

Date / Time	Talk 1	Lecturer
3. October 2011 11:10 - 11:45 + 5min. Discussion	Correlation effects in transport through quantum dots: renormalization-group approaches	Sabine Andergassen

Abstract

We investigate the effect of Coulomb interactions on the electronic transport through quantum dots. Using recently developed renormalization-group approaches, we present

i) an application to multi-level carbon nanotube quantum dots providing theoretical understanding for recent experiments. The observed bending of the Kondo ridges at finite magnetic field with respect to the ones at zero field is traced back to the renormalization of the level-reservoir coupling strength.

ii) analytical results for the non-equilibrium transport and relaxation dynamics for a minimal model for a charge-fluctuating quantum dot. Exploring the entire parameter space we find a rich physical behavior in the stationary regime as well as in the time evolution characterized by voltage-dependent oscillations and a power-law decay.

F4102-N13

Date / Time	Talk 2	Lecturer
3. October 2011 11:50 - 12:15 + 5min. Discussion	Towards million atoms: Semi-empirical potentials and inner eigenvalue solvers	Martijn Marsman

Abstract

M. Marsman, G. Jordan, and G. Kresse

We present the work on two related schemes.

(i) the construction of charge densities for non-selfconsistent DFT calculations: Effects of charge transfer are added onto the density of overlapping atomic charge densities by means of charge neutral spherical atom-centered Gaussian charge distributions that have been fitted to the self-consistent charge density in amorphous model systems.

(ii) We show that a combination of the Generalized Davidson method and harmonic Ritz values is well-suited for solving large interior eigenvalue problems: In many cases it is sufficient to calculate a few selected eigenstates of the system (for instance, a limited number of states near the valence and conduction band edges, and defect states within the forbidden gap).

F4103-N13	Date / Time	Talk 3	Lecturer
	3. October 2011 14:00 - 14:25 + 5min. Discussion	Optical conductivity with Wannier orbitals	Philipp Wissgott
	Abstract		
	Affiliation: Institute for Solid State Physics, Technical University Vienna, Austria We present an algorithm to compute the optical conductivity of materials within the LDA+DMFT framework by use of Wannier orbitals. In particular, we provide insights to a new way to use group velocities beyond the standard Peierls approximation directly computed within the underlying LDA calculation. Instead of direct derivatives of the band energies, these dipole matrix elements often lead to a better description of optical excitations, especially when the system contains both localized and itinerant electrons. Focusing on the technical details of the algorithm, the k-integration is often crucial and usually has to be chosen very carefully from case to case. In this new implementation, the k-mesh adaptively refines to resolve important features in k-space depending on the individual material. Therefore, the method can be applied to a wide range of compounds from strong to weak correlation effects. As an example of an application to physical systems of interest, we show results from the strongly correlated perovskite SrVO$_3$. Collaborators: J. Kunes, A. Toschi, K. Held		

F4104-N13	Date / Time	Talk 4	Lecturer
	3. October 2011 14:30 - 14:55 + 5min. Discussion	Cluster update for Tensor Network States	Ling Wang
	Abstract		
	We propose a new imaginary time evolution method for the 2 dimensional tensor network states. This method allows efficient simulation of the ground states admitting long range entanglement and large unit cell. We benchmark our method with the antiferromagnetic spin 1/2 Heisenberg model and the stagger dimerized Heisenberg model on square lattice. We observe significant improvements on energy and antiferromagnetic magnetization over the simple update. I will also present results for the frustrated Heisenberg model.		

Guest Lecture	Date / Time	Talk 5	Lecturer
	3. October 2011 15:30 - 16:05 + 5min. Discussion	Stacking Fault Energies in Austenitic Steels from Density Functional Theory	Peter Puschnig
	Abstract		

Peter Puschnig,
Chair of Atomistic Modelling and Design of Materials, Montanuniversität Leoben

FeMn-based austenitic steels have attracted great interest due to their superior ductility and strength under mechanical stress. Their deformation behavior has been related to the magnitude of the stacking fault energy (SFE) which is defined as the energy difference between the ideal fcc structure and the intrinsic stacking-fault structure. The former has ...ABCABCABCA... stacking along the [111] direction, while the latter exhibits a single planar defect that changes the fcc stacking into ...ABCAB|ABCA..., due to the slip of Shockley partial dislocations along the [112] direction. When the SFE is smaller than 20 mJ/m2, a process called transformation induced plasticity (TRIP) is observed, whereas for larger SFEs, twins are formed in twinning induced plasticity (TWIP). Measurements of the SFE are, however, cumbersome and scarce, which has motivated its calculation using thermodynamic approaches as well as ab-initio electronic structure calculations.

In this presentation, it will be outlined how the SFE can be calculated from density functional theory. First, it is shown how interstitial carbon atoms influence the SFE by employing a super cell approach within an all-electron full-potential framework. Second, the influence of Mn-concentration and temperature on the SFE in FeMn alloys is discussed. To this end, chemical and magnetic disorder are treated within the coherent potential approximation (CPA) and the disordered local moment (DLM) theory, respectively. The importance of temperature dependent magnetic moments and their contribution to the entropy is emphasized leading to composition and temperature dependent SFEs in good agreement with available experimental data.

	Date / Time	Talk 6	Lecturer
F4105-N13	3. October 2011 16:10 - 16:35 + 5min. Discussion	Towards an accurate description of the electronic properties of graphene defect structures	Hasan Pašalić

Abstract

Hasan Pašalić, Florian Libisch, Rafael Reiter, Joachim Burgdoerfer, and Hans Lischka

We aim at calculating electronic properties of ideal and defective (chemical substitution and adsorption, vacancies, etc.) mesoscopic, one- and two-dimensional carbon-based devices. To capture both the strong correlation in the □-conjugated polycyclic aromatic compounds, and to effectively treat large devices, we combine highly accurate ab initio methods with computationally effective empirical approaches able to handle millions of atoms. High-level quantum chemistry methods, such as complete active space self-consistent field (CASSCF) and multireference averaged quadratic coupled cluster (MR-AQCC) are used to account correctly for the potentially multiradical character of these systems. The quantum chemical results are then used to fit tight binding (TB) parameters. Using a geometry-dependent TB formulation with 8 spin orbitals for each carbon atom allows us to obtain a transferable tight-binding parametrization that can be used to calculate the local electronic structure of large-scale carbon-based nanodevices, and their transport properties. We present the current status and give a brief outlook.

F4106-N13	Date / Time	Talk 7	Lecturer
	3. October 2011 16:40 - 17:05 + 5min. Discussion	Handling continua in time-dependent external fields	Armin Scrinzi
	Abstract		
	The wave-function description of photo-electrons in the presence of non-perturbatively strong external fields requires very large simulation volumes to avoid reflections from box boundaries. It will shown that such wave functions can be truncated without introducing any distortions using "infinite range exterior complex scaling" (irECS). In spite of the truncation, exact photo-electron momentum spectra can be computed by analyzing the time-depedent surface flux (t-SURFF). Examples for the description of atoms and surface emission will be discussed.		

F4107-N13	Date / Time	Talk 8	Lecturer
	3. October 2011 17:10 - 17:35 + 5min. Discussion	Calculation of NMR Chemical Shifts in APW based methods	Robert Laskowski
	Abstract		
	We will present our implementation of the NMR chemical shift calculations within the APW-based methods. Until now calculations of NMR shifts in solids were performed mainly within plane-wave pseudo-potential methods and a PAW reconstruction of the all-electron wave functions.[1-3] Therefore we focus on the differences between the APW and pseudo-potential formalism, which are related to the APW representation of the wave function (inside the atomic spheres) and the representation of the current density. We will also discuss certain aspects related to the basis set enhancement for unoccupied states, which are necessary to obtain converged calculations. Finally we will present some results of NMR shifts validating our implementation. F. Mauri, B. G. Pfrommer, S. G. Luie, PRL 77, 5300 (1996) C. J. Picard, F. Mauri, PRB 63, 245101 (2001) J. R. Yates, C. J. Picard, F. Mauri, PRB 76, 024401 (2007)		

F4109-N13 / 1	Date / Time	Talk 9-1	Lecturer
	3. October 2011 17:40 - 17:52	Spin order calculations for $LaMnO_3$	Christoph Gruber
	Abstract		
	(P09, Peter Mohn, supervisor) The pseudo-binary system (La-Sr)MnO_3 shows a multitude of magnetic properties ranging from simple ferromagnetism to non-collinear magnetic order. Connected to these magnetic features is a structural phase transition from cubic to orthorhombic at the La-rich compositions. We use the VASP code to calculate non-collinear spin ordering for $LaMnO_3$ within the framework of LDA+U.		

F4109-N13 / 2

Date / Time	Talk 9-2	Lecturer
3. October 2011 17:53 - 18:05 + 5min. Discussion	Quantum Monte Carlo - Stochastic Series expansion, application to NMR spectra.	Robert Achleitner

Abstract

(Peter Mohn and Hans Gerd Evertz supervisors)
CMS TU Wien und TU Graz

The motivation of this work is to apply our QMC algorithm to a realistic problem. We use the Quantum-Monte-Carlo algorithm Stochastic Series Expansion for low dimensional spin systems in the spin1/2-Heisenberg model.

The systems we are investigating are spin-ladder compounds containing impurity sites. In experiment it is found that their NMR-Spectra show a significant broadening upon decreasing temperature as compared to systems without impurities. During the presentation it will be explained how to obtain NMR spectra out of such a QMC simulation and our achieved results will be shown.

Guest Lecture

Date / Time	Talk 10	Lecturer
4. October 2011 09:00 - 09:35 + 5min. Discussion	Multiscale computational tribology	Andras Vernes

Abstract

A. Vernes[1,2]

[1]Austrian Center of Competence for Tribology, Viktor-Kaplan-Straße 2, A-2700 Wiener Neustadt, Austria

[2]Institute of Applied Physics, Vienna University of Technology, Wiedner Hauptstr. 8 -10/ 134, A-1040 Vienna, Austria

Tribological processes, e.g. friction and wear, are multiscale phenomena in their nature, i.e. hierarchical in length and time. Therefore tribological systems can be realistically modelled/simulated only in a multiscale fashion, namely by coupling various computational methods, which are highly accurate on their typical length/time scales. Main computational parts of such a multiscale tribological calculation are based on quantum mechanics (QM), molecular dynamics (MD), continuum mechanics (CM) and multibody system dynamics (MBSD), respectively. Although length and time scales overlap to some extent when passing from a computational part to the immediately next one, the main challenge of the multiscale computational tribology still remains the coupling between different levels of modelling.

In the present talk, firstly, some of the well-established approaches and known methods will be extended and used to understand important tribological mechanisms on their relevant time/length scales. Secondly, some of these techniques which are proper on a given scale will be combined into new schemes to cover the hierarchical aspects of various tribological processes.

F4110-N13

Date / Time	Talk 11	Lecturer
4. October 2011 09:40 - 10:05 + 5min. Discussion	Progress Report on the Subproject P10: Cluster Expansion	Raimund Podloucky

Abstract

We report about latest results, developments and problems of applying the Cluster Expansion for the study of concentration dependent physical properties of alloys. Results on the binary Fe$_x$Al$1-x$ system will be discussed in more detail.

Guest Lecture

Date / Time	Talk 12	Lecturer
4. October 2011 10:40 - 11:15 + 5min. Discussion	Multi-scale modelling of high-temperature magnetization dynamics.	Oksana Chubykalo-Fesenko

Abstract

O.Chubykalo-Fesenko[1], U.Atxitia[1], D.Hinzke[2], U.Nowak[2], R.Evans[3], R.W.Chantrell[3]

1Instituto de Ciencia de Materiales de Madrid (CSIC), Spain

2University of Konstanz, Germany

3University of York, UK

Multiple recent applications (heat-assisted magnetic recording, laser-induced magnetization dynamics, thermally-assisted domain wall motion etc.) are related to temperature dependent magnetization dynamics. For this purpose we suggest the use of a hierarchical multi-scale scheme [1]. First, the generalized Heisenberg Hamiltonian is parameterized via the ab-initio calculations. Next, we have developed several methods to evaluate temperature dependence of macroscopic parameters such as the macroscopic anisotropy [2] or the exchange stiffness [3]. Finally, these parameters are used as an input to large-scale micromagnetic modelling based on the Landau-Lifshitz-Bloch equation [1]. As an example, we will consider laser-induced magnetization dynamics when the temperature is often raised above the Curie temperature. We will present our recent results on modelling in Ni [4] and Gd [5] and compare them with experiments. The magnetization dynamics in Ni is quenched on the fs timescale and recovered on the timescale of 10 ps. Gd presents two-step demagnetization where the magnetization recovery occurs in 100 ps. We will also present some recent results on modelling of magnetization switching in a ferromagnetic compound CoFeGd.

References:

[1] N.Kazantseva et al Phys. Rev. B 77 (2008) 184428

[2] P.Asselin et al Phys. Rev. B 82 (2010) 134440

[3] U.Atxitia et al Phys. Rev. B 82 (2010) 054415

[4] U.Atxitia et al Phys. Rev. B 81 (2010) 174401

[5] U.Atxitia and O.Chubykalo-Fesenko Phys. Rev. B (2011)

F4112-N13

Date / Time	Talk 13	Lecturer
4. October 2011 11:20 - 11:45 + 5min. Discussion	Accelerated Langevin simulations for calculating rare switching events using Forward Flux Sampling	Christoph Vogler

Abstract

Predicting the thermal stability of magnetic storage devices is an important and challenging task. In the presented work, we developed a technique consisting of a combination of a nudge elastic band (NEB) [1][2] method, which is part of our finite element micromagnetic package FEMME, and a statistical method to simulate rare events called “Forward Flux Sampling” (FFS) [3] method. With this technique it is possible to calculate the attempt frequency of single domain particles as well as for fully micromagnetic models under arbitrary homogeneous external fields. Along the minimum energy path obtained by the NEB a set of interfaces can be defined. Langevin dynamic calculations (a stochastic random field is added to the Gilbert equation) are performed to calculate the probability that the magnetization sate of the system passes from interface i to interface i+1. If all the transition probabilities between the interfaces are known the average lifetime of the particle can be calculated. Real memory bits have typical thermal longtime stabilities of 20-30 year, which cannot be simulated with standard Langevin dynamic simulations. With the FFS approach it is possible to extract these lifetimes out of several simulations in the nanosecond scale to the time scale of years.

References:

[1] G. Henkelman et al, Improved tangent estimate in the nudged elastic band method for finding minimum energy paths and saddle points, The Journal of Chemical Physics 133(22), 9978, 2000

[2] R. Dittrich et al, A path method for finding energy barriers and minimum energy paths in complex micromagnetic systems, Journal of Magnetism and Magnetic Materials 250, 12–19, 2002

[3] R.J. Allen et al, Sampling Rare Switching Events in Biochemical Networks, Physical Review Letters 94(1), 018104, 2005

[4] W.T. Coffey et al, Effect of an oblique magnetic field on the superparamagnetic relaxation time; Influence of the gyromagnetic term, Physical Review B 58(6), 3249, 1998

F4111-N13

Date / Time	Talk 14	Lecturer
4. October 2011 11:50 - 12:15 + 5min. Discussion	Factors contributing to the glass-forming ability of a simulated molecular liquid	Ulf Rørbæk Pedersen

Abstract

	When liquids are cooled, they may solidify into two quite different phases: a crystal phase with long-range order or an amorphous glassy phase. Understanding this competition constitutes an important problem in condense matter physics fields such as metallic glasses, pharmacology, crystal engineering and nanotechnology. Perhaps the most common strategy for optimizing glass forming ability is to look to increasing the thermodynamic stability of the liquid with respect to the crystal phase. In general, however, also slow liquid dynamics and the crystal-liquid interphase may play an important role. Here, we investigate a liquid of Lennard-Jones trimers, inspired by ortho-terphenyl, originally suggested as a good glass former [Lewis and Wahnstrom, 1993]. In micro seconds simulations, however, the liquid crystallize into a structure where the three spheres that make up the rigid molecule sit near the sites of a body centered cubic lattice. The trimer bond angle is almost optimal for this structure. The maximum crystallization rate, in reduced units, is 10^4 times slower than the Lennard-Jones liquid. We present evidence that this enhanced glass forming ability is due, in equal parts, to slower liquid dynamics and a larger crystal-liquid interfacial free energy in the molecular liquid.