Thursday, April 4th 2013			
Time	**Talk**	**Lecturers**	**Details**
10:00 – 10:15	*Greetings*	**Georg Kresse**	15 min.
10:15 – 11:00	*Probing a Liquid to Glass Transition in Equilibrium*	**Walter Kob**	Guest Lecture 45 min.
11:00 – 11:30	Coffee Break (30 min.)		
11:30 – 12:10	*Self-assembly of heterogeneously charged particles under confinement*	**Emanuela Bianchi**	P11 40 min.
12:10 – 12:50	*Efficient RPA calculations using Green functions*	**Merzuk Kaltak**	P02 40 min
12:50 – 13:50	Lunch (60 min.)		
13:50 – 14:30	*Bound states and "Quantum Bowling"*	**Hans Gerd Evertz**	P04 40 min.
14:30 – 15:10	*Cluster expansion study of the Ni-Pt alloy system*	**Martin Leitner**	P10 40 min.
15:10 – 15:40	Coffee Break (30 min.)		
15:40 – 16:10	*Hybrid-DFT with an optimized mixing parameter*	**David Koller**	P07 30 min.
16:10 – 16:40	*Covalent magnetism and magnetic impurities*	**Christoph Gruber**	P09 30 min.
16:40 – 17:10	*Spin-orbit coupling induced effects in practical antiferromagnets and new route in antiferromagnetic spintronics.*	**Sergeii Khmelevskyi**	P09 30 min.
17:10 – 18:10	General Meeting (ViCoM-Members Only, 60 min.) Seminarraum 3		
18:10 – 20:10	Dinner Buffet *UniBräu Kellerstüberl* (120 min.)		

Friday, April 5th 2013			
Time	**Talk**	**Lecturers**	**Details**
09:00 – 09:45	*Optical and vibrational properties of 2D materials with ab-initio techniques*	**Ludger Wirtz**	Guest Lecture 45 min.
09:45 – 10:25	*Calculations of the F-center in LiF*	**Paul Tiwald** **Ferenc Karsai**	P05 & p07 40 min.
10:25 – 10:55	Coffee Break (30 min.)		
10:55 - 11:40	*Superconductivity, a Computational Approach*	**Lilia Boeri**	Guest Lecture 45 min.
11:40 – 12:20	Relative entropy measures for correlations	**Norbert Mauser**	P06 40min.
12:20 – 14:00	Lunch at *Culinarium Cooking* (100 min.)		
14:00 -14:40	*Steady-State Nonequilibrium Dynamical Mean Field Theory: an auxiliary Lindblad Master Equation approach*	**Enrico Arrigoni**	P03 40 min.
14:40 – 15:20	*Fast Convolution Method for non-uniform data*	**Lukas Exl**	P12 40 min.
15:20 – 15:50	Coffee Break (30 min.)		
15:50 – 17:20	Discussion (90 min.)		
17:20 – 17:30	*Farewell*	**Georg Kresse**	10 min.

Guest Lectures

Friday, April 5th 2013 – 11:05 p.m.	
Lilia Boeri *Graz University of Technology*	***Superconductivity, a Computational Approach*** Superconductivity is one of the oldest and most fascinating problems in solid state physics. In the last ten years, the advancement of ab-initio techniques has permitted to gain a deep insight into the material-dependent properties which characterise real superconductors, and in some cases to anticipate trends in new materials. In my talk, I will review a few recent examples, starting with the classical BCS example of intercalated graphites, and moving on to more controversial cases, such as iron-based superconductors and organic compounds.

Thursday, April 4th 2013 – 10:15 a.m.	
Walter Kob *Université Montpellier 2*	***Probing a Liquid to Glass Transition in Equilibrium*** A glass is an amorphous solid formed by cooling a glass-forming liquid below the experimental glass temperature. Although certain theoretical approaches predict that this dynamical arrest is related to a thermodynamic transition, such a singularity must occur in a temperature regime where it is impossible to do experiments under equilibrium conditions. Recently a new method has been proposed that should make it possible to probe the equilibrium properties of a glass-former even at its Kauzmann temperature. In this talk I will present this method and discuss first results of computer simulations that give evidence that at the Kauzmann point the system undergoes a first order phase transition from a liquid to an ideal glass state.

Thursday, April 5th 2013 – 09:00 a.m.	
Ludger Wirtz *University of Luxembourg*	***Optical and vibrational properties of 2D materials with ab-initio techniques*** Besides graphene, other (quasi)2D materials such as hexagonal boron nitride (hBN) and molybdenum disulfide (MoS2) are receiving increased attention recently. Many groups are performing optical and vibrational spectroscopy on these materials. Since the layer is usually in contact with a substrate, the chemical/physical interaction with the substrate and/or the dielectric screening by the substrate can substantially alter the properties. I will give a few examples how ab-initio methods (GW, Bethe-Salpeter, density-functional perturbation theory) help to understand the subtle changes in the optical and vibrational properties of 2D layered materials due to the influence of the environment.

Project Parts Presentations

Thursday, April 4th 2013 – 12:10 p.m.	
Merzuk Kaltak P02 - *Towards Exact Correlation in Extended Systems* PI/Project Leader: **Georg Kresse**	***Efficient RPA calculations using Green functions*** The computationally most expensive step in *GW* and RPA implementations is the calculation of the independent particle polarizability χ. We present an RPA code that calculates χ using the Green function *G* in real space and imaginary time. The systematic construction of optimized time and frequency grids for G is obtained by means of solving a fitting problem. Furthermore a non-uniform discrete Fourier transform between the two grids is introduced, which converges exponentially. We show that the usage of the Green function approach in combination with the optimized grids can be used for the calculation of the RPAcorrelation energy for very large systems. In addition aspects of a corresponding real-space-imaginary-time *GW* implementation are discussed.

Friday, April 5th 2013 – 02:00 p.m.	
Enrico Arrigoni P03 - *Dynamical Mean Field Theory & Beyond* PI/Project Leader: **Karsten Held** Research/National Partner: **Enrico Arrigoni**	***Steady-State Nonequilibrium Dynamical Mean Field Theory: an auxiliary Lindblad Master Equation approach*** We present a method to compute electronic steady state properties of strongly correlated quantum systems out of equilibrium within dynamical mean-field theory (DMFT). The DMFT solver is based on the exact solution of an auxiliary system consisting of a small number of bath sites coupled to the interacting impurity and to two Markovian reservoirs. The steady state Green's function of the auxiliary system is solved by exact diagonalisation of the corresponding many-body Lindblad equation. The approach can be regarded as the non-equilibrium extension of the exact-diagonalization based DMFT.

Thursday, April 4th 2013 – 12:50 p.m.	
P04 - *Quantum Impurity Solvers* PI/Project Leader: **Frank Verstraete** Research/National Partner: **Gerd Evertz**	***Bound states and "Quantum Bowling"*** Bound states in strongly correlated systems like the Heisenberg spin chain have been difficult to detect experimentally. We discuss a nonequilibrium setup in which these states become prominent during the time evolution after a local quantum quench, which we calculate by time dependent DMRG. They persist even when integrability breaking perturbations are included. The setup is realizable in cold atom experiments. The second part of the talk will introduce "Quantum Bowling", the scattering of propagating soliton-like particles from a wall of bound particles, in the XXZ model and the 1d Bose and Fermi Hubbard models. We show that there is a simple but very surprising pattern of scattering, very different from classical behavior. Potential applications will be discussed, including a fermionic Quantum Newton's cradle.

Friday, April th 2013 – 09:45 a.m.		
Paul Tiwald P05 - *Embedded Cluster Approach & Non-Adiabatic Processes in Physics & Chemistry* PI/Project Leader: **Joachim Burgdörfer** Research/National Partner: **Hans Lischka**	**Ferenc Karsai** P07 - *Electronic Structure of Solids, Surfaces & Nanostructures* PI/Project Leader: **Peter Blaha**	***Calculations of the F-center in LiF*** We present a joint study of the project parts #5 and #7 on the F-type color-center in LiF. This is an old prototype problem where an electron is trapped at a vacant anion site. In an intuitive picture the defect electron can be approximately described as a particle in the box. We present a comparison of the physicist's approach (periodic supercell-approach with various DFT-functionals, GW and Bethe-Salpeter methods) and the quantum-chemist's approach (embedded-cluster approach with wave-function methods such as CASPT2). In both cases, we observe strong excitonic effects due to the strong localization of the defect in agreement with the simple particle in box picture. We discuss the advantages and limitations of both methods and compare their performance on a quantitative level.

Frieday, April 5th 2013 – 11:55 a.m.	
Norbert Mauser P06 - *Dynamical Correlated Systems* PI/Project Leader: **Norbert Mauser** Research/National Partner: **Armin Scrinzi**	***Relative entropy measures for correlations***

Thursday, April 4th 2013 – 03:10 p.m.	
David Koller P07 - *Electronic Structure of Solids, Surfaces & Nanostructures* PI/Project Leader: **Peter Blaha**	***Hybrid-DFT with an optimized mixing parameter*** Usually in (screened) hybrid functionals the fraction alpha of Hartree-Fock exchange is kept fixed in a certain parametrization. However there is no single (universal) value for alpha which systematically leads to a satisfying accuracy for very different systems like semiconductors or large band gap insulators. We use the static dielectric constant to determine alpha for a specific system in a self-consistent procedure and present results for the band gap and lattice constant of various semiconductors and insulators.

Thursday, April 4th 2013 – 04:10 p.m.	
Christoph Gruber P09 - *Complex Magnetic Structures* PI/Project Leader: **Peter Mohn** Research Partner/ National Partner: **Josef Redinger**	***Covalent magnetism and magnetic impurities*** We use the model of covalent magnetism and its application to magnetic insulators applied to the case of insulating carbon doped $BaTiO_3$. Since the usual Stoner mechanism is not applicable we study the possibility of the formation of magnetic order based on a mechanism favoring singly occupied orbitals. On the basis of our model parameters we formulate a criterion similar to the Stoner criterion but also valid for insulators. We describe the model of covalent magnetism using a molecular orbital picture and determine the occupation numbers for spin-up and spin-down states. Our model allows to simulate the results of our *ab-initio* calculations for E ($\mathcal{M}$) which are found to be in very good agreement

Thursday, April 4th 2013 – 04:40 p.m.	
Sergeii Khmelevskyi P09 - *Complex Magnetic Structures* PI/Project Leader: **Peter Mohn** Research Partner/ National Partner: **Josef Redinger**	***Spin-orbit coupling induced effects in practical antiferromagnets and new route in antiferromagnetic spintronics.*** The magnetic anisotropy energy (MAE) and element-specific contributions to the MAE have been studied for Mn-based antiferromagnetic alloys with layered $L1_0$ structure within the framework of the local spin-density approximation and the fully relativistic torque method. It is found that the contribution to the total MAE from nonmagnetic 3*d* and 4*d* elements in MnIr, MnNi and MnPd ordered alloy is determined not only by Mn contribution but also by strong spin-orbit coupling on non-magnetic transition metal atom. In addition we observe a strong dependence of the MAE on the state of magnetic order [1]. This effect appears to be due to competition between in-plane and uniaxial atomic specific contributions from Mn and transition metal atoms to the MAE. The switching of the magnetization in considering AFM materials may lead to the giant change in the magnetoresistance and thus it may proposed a new route in antiferromagnetic spintronics The idea is to control the magnetization reversal in antiferromagnets via the changing the c/a ratio in antiferromagnetic thing films [2]. We illustrate this idea by calculating the respective anisotropic changes in the relativistic Density of State of in novel high temperature Mn_2Au antiferromagnetic compound [3] and MnIr alloy. [1] S. Khmelevskyi, A. B. Shick, and P. Mohn, Phys. Rev. B **83**, 224419 (2011). [2] A. B. Shick, S. Khmelevskyi, O. N. Mryasov, J. Wunderlich, and T. Jungwirth, Phys. Rev. B 81, 212409 (2010). [3] S. Khmelevskyi, and P.Mohn, Appl. Phys. Lett. 93, 162503 (2008).

Thursday, April 4th 2013 – 02:30 p.m.	
Martin Leitner P10 - *Multi-Scale Simulations of Multi-Component Phases* PI/Project Leader: **Raimund Podloucky** Research/National Partner: **Jürgen Hafner** **Ernst Kozeschnik**	***Cluster expansion study of the Ni-Pt alloy system*** The cluster expansion (CE) is a state-of-the-art tool for exploring the configuration space of multi-component systems with the accuracy of density functional theory (DFT) calculations. Based on the figure set of a converged CE Monte-Carlo (MC) simulations are performed in order to derive temperature dependent phase stabilities. This CE+MC approach - as implemented in the UNCLE package [1] - is applied to study the Ni--Pt alloy system, for which the formation of ordered phases at low temperatures is under debate. DFT studies focused on three ordered phases, namely $NiPt_3$ and Ni_3Pt with $L1_2$ structure and NiPt with $L1_0$ structure. A CE study predicted an additional stable Pt-rich phase of $NiPt_7$ composition, which was not confirmed by recent DFT studies and experiment. A further DFT study predicted a Ni-rich Ni_3Pt phase with $D0_{22}$ ordering to be energetically more favorable than the $L1_2$ structure. Based on DFT calculations performed with VASP an extensive CE+MC study was done for the whole composition range. The results will be critically compared to the existing data. Furthermore, calculated short range order intensities are compared to very recent X-ray Photon Correlation Spectroscopy (XPCS) experiments in the Ni-rich regime. [1] D. Lerch et al., Modelling Simul. Mater. Sci. Eng. **17** (2009), 055003

Thursday, April 4th 2013 – 11:30 a.m.	
Emanuela Bianchi P11 - *Nucleation & Self-Assembly in Soft Matter Systems: From the Molecular to the Mesoscopic* PI/Project Leader: **Christoph Dellago** Research/National Partner: **Gerhard Kahl**	***Self-assembly of heterogeneously charged particles under confinement*** We consider axially symmetric quadripolar colloids in a confined planar geometry and study the role of both the overall particle charge and the patch extension as well as the effect of a neutral or possibly charged substrate. A general tendency to form quasi two-dimensional aggregates where particles align their symmetry axes within the plane is found; a clear distinction between the formation of microcrystalline gels -- branched networks consisting of purely crystalline domains -- as opposed to disordered aggregates can be observed based on the specific features of the particle-particle interaction. Additionally, the possible competition of interparticle and particle-substrate interactions affects the size and the internal structure of the aggregates and can possibly inhibit the aggregation process.

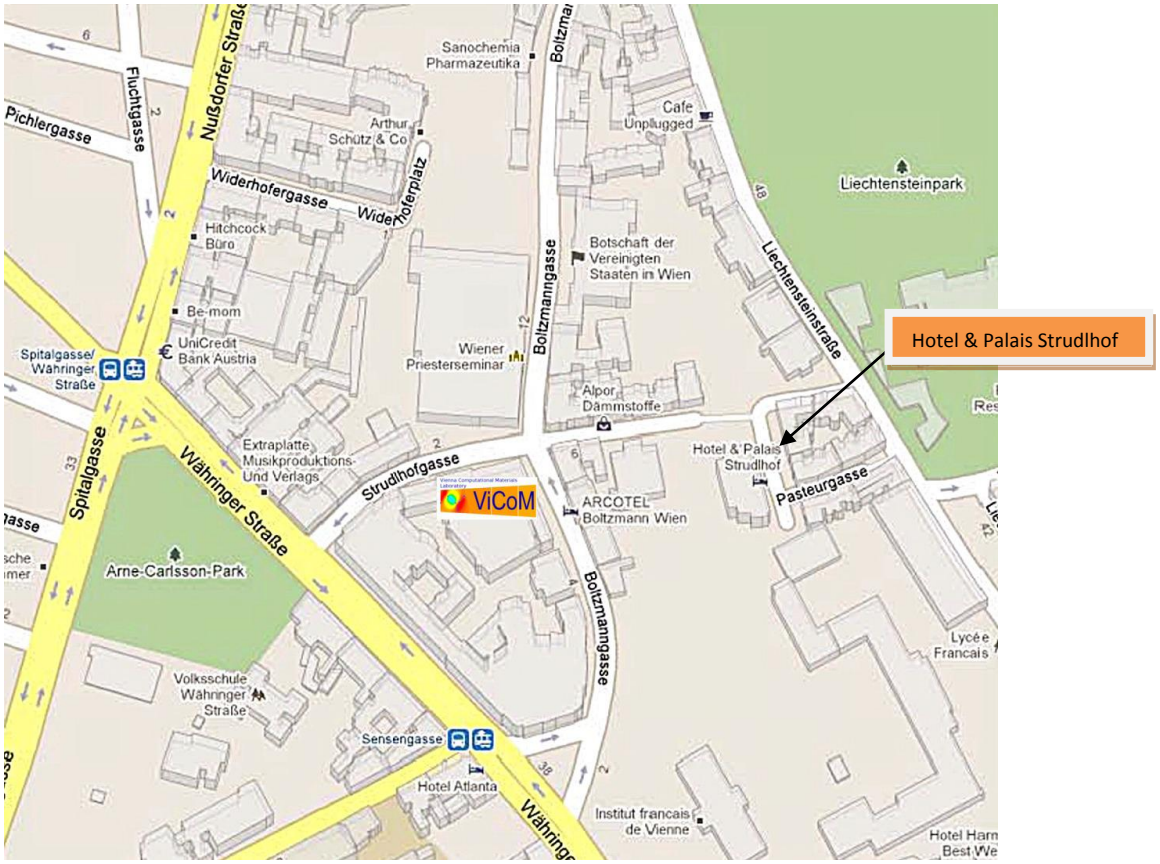
Friday, April 4th 2013 – 02:40 p.m.	
Lukas Exl P12 - *Multi-Scale Simulations of Magnetic Nanostructures* PI/Project Leader: **Dieter Suess** Research/National Partner: **Thomas Schrefl**	***Fast Convolution Method for non-uniform data*** Directly computed convolution for arbitrary located M sources and N targets scales $\mathcal{O}(MN)$. We present a fast method based on non-uniform discrete Fourier transform (NUDFT) that scales $\mathcal{O}(n^d \log(n) + M + N)$, where n is the mesh size of an auxiliary tensor grid and d the space dimension. The method is extended to handle a large class of singular kernel functions, e.g. Green functions from potential theory. In addition we present a new methodology that further reduces the costs by structured tensor approximation.

Basic Information

Venue

All lectures take place at "Christian-Doppler-Hörsaal" at Strudlhofgasse, 3rd floor, 1090 Vienna. For instructions on how to get there visit http://physik.univie.ac.at/lageplan-kontakt/lageplan/. The lecture hall is well equipped (1 video-projector, 1 overhead-projector, 2 screens, 1 blackboard, 1~2 multiple sockets as temporary charging stations for laptop batteries, WLAN access via *eduroam* (you can also ask Katharina Simma for a temporary ID).

ote: If you want to work with your laptop during the workshop, please make sure that the batteries are charged before you enter the lecture hall – Due to a security advice regarding the capacity of the busbars in the lecture hall, we must not use more than 1~2 multiple sockets coevally in the lecture hall. Thank you for your understanding.



ID Badge

When you arrive at the location, please pick up your ID badge and sign in before entering the lecture hall. Keep your ID badge clearly visible at all times (especially during the coffee-breaks and during the meals). Finally, please do not forget to return your ID badge before you leave. Thank you in advance.

Coffee Breaks & Thursday Lunch

The coffee breaks and Thursday lunch will take place in the anteroom of the lecture hall. Food and drinks are for free, but for registered attendees only. Please keep your ID badge clearly visible at all times. Thank you in advance.

Dinner

The dinner on Thursday will take place in the *Universitätsbräuhaus*. Food and drinks are free, but for registered attendees only. Please keep your ID badge clearly visible at all times.
Universitätsbräuhaus
Campus of the University of Vienna (Hof 1)
Alserstraße 4
A-1090 (9th District)
For information on how to get there visit: http://www.unibrau.at/.

Friday Lunch

The lunch on Friday will take place in the *Culinarium Cooking Restaurant*. Food and drinks are free, but for registered attendees only. Please keep your ID badge clearly visible at all times.
Culinarium Cooking Restaurant Währinger Straße 21, A-1090 Vienna.