Vienna Computational Materials Laboratory

ViCoM

ViCoM WORKSHOP APRIL 2011 / Programme & Schedule

28.04.2011 – 29.04.2011

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PROGRAMME

PROJECT PART 02: "TOWARDS EXACT CORRELATION IN EXTENDED SYSTEMS"

Principal Investigator / Project Part Leader: Georg Kresse

Project Part	Date & Time	Presentation
P02	Thursday, 28.04.2011, 13:30 – 14:00	**"Self-consistent RPA Potential via the Sham Schlüter Equation"** (Georg Kresse, 25-30 min.)
	RPA and GW calculations are usually performed non-selfconsistent using the Kohn-Sham orbitals and determining the change in the one electron energies using first order perturbation theory (LDA+GW). Two methods can be used to remedy this restriction. Schilfgaarde and Kotani suggested a selfconsistent GW approach. Alternatively a local multiplicative Kohn-Sham potential can be calculated self-consistently within the random-phase approximation, and the QP energies can be determined using the conventional perturbational GW method (RPAKS+GW). *For most materials small improvements are found compared to conventional LDA+GW calculations, but for ``difficult'' systems, the predicted band gaps are in fact improved over the conventional LDA+GW approach.*	

MEMO

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
P03 / A	Thursday, 28.04.2011, 11:00 – 11:20	**"Iron-based Superconductors from an LDA+DMFT Perspective"** (Markus Aichhorn, 20 min.)
	The discovery of high-temperature superconductivity in iron-based compounds triggered an enormous amount of research in condensed matter physics. Not even two years after their discovery, scientist have already collected a huge amount of experimental data, due to very powerful experimental techniques that have been developed during the last decades. A very intriguing property of these new compounds is the rather high flexibility concerning elemental substitutions, leading to several families of superconductors, termed '1111', '122', '11', and so on, depending on their chemical composition. We analyse the single-particle properties of prominent iron-based superconductors using a combination of density-functional theory with a state-of-the-art many-body technique, the Dynamical Mean-Field Theory. This approach enables us to understand also these more complex materials at a first-principle level. We will show that there are significant differences in the electronic properties, when going from more weakly correlated members as LaFeAsO, to more correlated ones like FeSe. For reasonable Coulomb parameters, the properties range from Fermi-liquid like to incoherent bad-metal like.	

MEMO

Project Part	Date & Time	Presentation
P03 / B	Thursday, 28.04.2011, 11:20 – 11:40	**"Dynamical Vertex Approximation for Nanoscopic Systems"** (Angelo Valli, 20 min.)
	We present a general scheme to the calculation of finite-size complex network in the spirit of the recently introduced Dynamical Vertex Approximation (DΓA). We validate our approximation, at the single-particle level, against a numerically exact Quantum Monte Carlo for a multi-site Anderson Impurity Model for a reasonably small system. As a more pioneering application we propose a model for a quantum point contact made of about hundred correlated atoms; in agreement with experimental evidences, we observe a sharp drop of the conductance through the junction, which can be explained in terms of a local Mott-Hubbard crossover.	

MEMO

Project Part	Date & Time	Presentation
P03 / C	Thursday, 28.04.2011, 11:40 – 12:00	**"Wien2wannier: From Linearized Augmented Plane Waves to Maximally Localized Wannier Functions"** (Philipp Wissgott, 20 min.)
	We present wien2wannier, an interface between the full-potential linearized augmented plane wave package Wien2k and the wannier90 code for the construction of maximally localized Wannier functions. The workflow starting from wien2k is shown step by step, including possible usages of the Wannier orbitals obtained from wannier90. Describing the main features of the algorithm, we introduce, as a simple example, the case of SrVO3. We consider also a more elaborate example, FeSb2, which is a compound with interesting thermoelectric properties. For this low symmetric material, we illustrate the procedure of obtaining a locally diagonal Wannier basis set from a wien2k bandstructure. These real space orbitals provide a convenient basis for DMFT calculations. We will be thus able to shine light on the effect of electronic correlations in compounds with a mixed d- and p-manifold at the Fermi edge. *J. Kuneˇs, R. Arita, P. Wissgott, A.Toschi, H. Ikeda, K. Held Wien2wannier: From linearized augmented plane waves to maximally localized Wannier functions, Comp. Phys. Commun. 181, 1888 (2010).* *Contact: wissgott@ifp.tuwien.ac.at*	

MEMO

PROJECT PART 04: "QUANTUM IMPURITY SOLVERS"

Principal Investigator / Project Part Leader: Frank Verstraete Research Partner / National Partner: Hans Gerd Evertz

Project Part	Date & Time	Presentation
P04	Thursday, 28.04.2011, 14:00 – 14:30	**"Variational Optimization of the Numerical Renormalization Group"** (Iztok Pizorn, 25-30 min.)
	Authors: Iztok Pizorn & Frank Verstraete *We rephrase the numerical renormalization group (NRG) as a variational method with the cost function given by the sum of all the energies of the effective low-energy Hamiltonian. This allows systematic improvement of the spectrum obtained by NRG through sweeping. The ensuing algorithm has a lot of similarities to the density matrix renormalization group (DMRG) when targeting many states, and this synergy of NRG and DMRG combines the best of both worlds and extends their applicability. We illustrate this approach with simulations of a quantum spin chain and a single impurity Anderson model (SIAM) where the accuracy of the effective eigenstates is greatly enhanced as compared to the NRG, especially in the transition to the continuum limit.*	

MEMO

PROJECT PART 05: "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
P05	Thursday, 28.04.2011, 14:30 – 15:00	**"Charge Exchange Between a LiF Surface and a Proton: An Embedded Cluster Approach"** (Franz P. Tiwald, 25-30 min.)
	We apply high-level quantum chemistry methods such as the multi-configuration self-consistent field (MCSCF) and multi-reference configuration interaction (MRCI) approach to describe the interaction dynamics of a LiF surface with a proton. The strength of these methods lies in their ability to account for strong correlations of localized electrons. In our model the LiF surface is represented by a small active cluster which is embedded into a surrounding matrix mimicking the infinite system. The embedding scheme plays a crucial role to realistically describe the interaction of charged particles with the LiF surface. First results on the structure and dynamics will be presented.	

MEMO

PROJECT PART 06: "DYNAMICAL CORRELATED SYSTEMS"

Principal Investigator / Project Part Leader: Norbert J. Mauser Research Partner / National Partner: Armin Scrinzi

Project Part	Date & Time	Presentation
P06	Thursday, 28.04.2011, 15:30 – 16:00	**"MCTDHF: state of the art"** (Norbert J. Mauser, 25-30 min.)
	We present the Multic Configuration Time Dependent Hartree Fock equations and their extension to systems where the nuclei move according to classical dynamics. We present ongoing work both on the analysis of this complex system of coupled PDEs and ODEs and on the numerical methods used to solve them.	

MEMO

PROJECT PART 07: "ELECTRONIC STRUCTURE OF SOLIDS, SURFACES AND NANOSTRUCTURES"

Principal Investigator / Project Part Leader: Peter Blaha

Project Part	Date & Time	Presentation
P07	Thursday, 28.04.2011, 16:00 – 16:30	**"Results of Advanced DFT Functionals with WIEN2k"** (Peter Blaha, David Koller, 25-30 min.)
	We will present results for cohesive energies of molecules, lattice parameters of solids, surface energies as well as CO adsorption energies using our newly developed HTBS-GGA functional. Overall this GGA outperforms PBE and can also break (to some extend) the usual GGA-trend that GGAs with small errors for the surface energy have large errors for the CO adsorption energy. We will also present briefly the implementation of (screened) hybrid functionals in WIEN2k and finally analyze the performance of the TB-mBJ potential for band gaps, magnetic moments and EFGs in various transition metal compounds.	

MEMO

PROJECT PART 09: "COMPLEX MAGNETIC STRUCTURES"

Principal Investigator / Project Part Leader: Peter Mohn Research Partner / National Partner: Josef Redinger

Project Part	Date & Time	Presentation
P09	Thursday, 28.04.2011, 16:30 – 17:00	**"Magnetic Order in BaTiO3-xMx (M=C,N,B); the Search for Magnetic High Permittivity Materials."** (Christoph Gruber, 25-30 min.)
	C. Gruber, P. O. Bedolla-Velazquez, J. Redinger and P. Mohn *We present VASP calculations using the HSE functional for carbon, nitrogen, and boron doped BaTiO3-xMx (M=C,N,B). We calculate a 40-atom supercell replace one oxygen atom by C,N, or B. For all three substituents we find a magnetically ordered ground state which is insulating for C and N and halfmetallic for B. The changes in the electronic structure between the undoped and the doped case are dominated by the strong crystal field effects together with the large band splitting for the impurity p-bands. Using an MO picture we give an explanation for the dramatic changes in the electronic structure between the insulating non-magnetic state and the as well insulating magnetic state for C doped BaTiO3. The calculated optical properties show pronounced changes upon doping. p-element doped perovskites could provide a new class of materials for multi-ferroics applications.*	

MEMO

PROJECT PART 10: "MULTI-SCALE SIMULATIONS OF MULTI-COMPONENT PHASES"

Principal Investigator / Project Part Leader: Raimund Podloucky Research Partner / National Partner: Jürgen Hafner, Ernst Kozeschnik

Project Part	Date & Time	Presentation
P10 / A	Friday, 29.04.2011, 10:50 – 11:20	**"First-principles Study of the $Fe_xNi_yAl_{1-x-y}$ Alloy System by the Cluster Expansion"** (Martin Leitner, 25-30 min.)
	G. Kastlunger, M. Leitner, D. Reith, R. Podloucky – Institute for Physical Chemistry, Univ. Vienna *Cluster expansion (CE) is the state of the art tool to calculate phase diagrams of two or more constituents with DFT precision. In this presentation, we apply CE for a ternary system studying the $Fe_xNi_yAl_{1-x-y}$ alloy system. Because we are interested in the Fe-rich ternary alloys the CE is done for a bcc basic lattice. Utilizing VASP derived formation energies for selected atomic configurations the effective cluster interaction energies (ECI) are derived by employing the UNCLE (UNiversal CLuster Expansion) code of S. Müller and his group. After an extensive ground state search the stable phases in the bcc parent lattice were identified for the three possible binary and the ternary system. To construct the phase diagram at finite temperatures the ECIs were used in canonical as well as in grand canonical Monte Carlo calculations.*	

MEMO

Project Part	Date & Time	Presentation
P10 / B	Friday, 29.04.2011, 11:20 – 11:50	**"Analysis of the Influence of Vacancy-solute Interaction on Diffusion of Atomic Monomers and Clusters"** (Piotr Warczok, 25-30 min.)
	Authors: Piotr Warczok[1], Jaroslav Zenisek[2], Ernst Kozeschnik[1] *1 – Institute of Materials Science and Technology, Vienna University of Technology* *2 – Materials Center Leoben Forschung GmbH* *We investigate the dependence of the diffusional mobility of single solute atoms as well as clusters of atoms on the vacancy-solute binding characteristics with the Monte Carlo (MC) method. Existing works, mainly based on first-principles calculations and atomistic simulations, are reviewed first. The results of our MC simulations are explored in the light of the atomic clusters movement. Finally, we propose a numerical method for incorporation of this movement and potential collisions of clusters in a precipitation kinetics framework.*	

MEMO

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	Friday, 29.04.2011, 13:40 – 14:10	**"Self-Assembling DNA-coated Colloids. A Simulation Study"** (Panagiotis E. Theodorakis, 25-30 min.)
	P. E. Theodorakis[1,2], G. Kahl[2], C. Dellago[1] *1 Faculty of Physics, University of Vienna, Vienna, Austria* *2 Institute for Theoretical Physics, Technical University of Vienna, Vienna, Austria* *Colloids (or other meso-sized particles) functionalized with single-stranded DNA (ssDNA) are increasingly used to create designed structures based on the specificity and reversibility of the hydrogen-bonding between two complementary strands of DNA. DNA-coated colloids hold in this way great promise as building blocks of complex self-assembling colloidal materials. By means of Monte Carlo (MC) simulations based on effective interparticle potentials, we study the phase behavior and the self-assembling of such systems. Exploring a large set of functionalities, densities, strand lengths, and temperatures we extend recent studies providing a theoretical understanding for future development and applications of these materials.*	

MEMO

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
P12	Friday, 29.04.2011, 14:10 – 14:40	**"Stray Field Computation on Tensor Grids"** (Lukas Exl, 25-30 min.)

L. Exl[1], T. Schrefl[1], F. Bruckner[2], D. Suess[2]

[1] University of Applied Sciences, Department of Industrial Simulation, A-3100 St. Pölten, Austria

[2] Vienna University of Technology, Institute of Solid State Physics , A-1040 Vienna, Austria

Computation of the magnetostatic field is the most time-consuming aspect in micro-magnetic simulations. This is usually done by evaluating the magnetostatic scalar potential, which involves the solution of a Poisson equation, e.g., by means of a hybrid FEM/BEM method, see e.g. [5]. Alternatively, direct computation by discretization of a volume integral formulation of the scalar potential normally scales with the total number of computational cells squared, i.e. O(n6) for n3 cells. We present an analytically-based tensor approximation method for computing the magnetostatic scalar potential and stray field, which can be generally used for a special class of function-related tensors [4]. Calculation of the scalar potential and the stray field reduces to multi-linear algebra operations, which can be implemented efficiently using optimized libraries [6], [1], [2]. The method scales almost linearly, i.e. O(n4) in the general case and superlinear, i.e., O(n2) for specially structured magnetization tensors, e.g. in the CP-format. Using canonical tensor formats could open up new possibilities for solving the LLG equation eciently by projection methods (e.g., CG or GMRES) for linear systems in tensor format, recently introduced in [3].

References

[1] B. W. Bader and T. G. Kolda. Algorithm 862: MATLAB tensor classes for fast algorithm prototyping. ACM Transactions on Mathematical Software (TOMS), 32:635{653, Dec. 2006. ACM ID: 1186794.

[2] B. W. Bader and T. G. Kolda. Ecient MATLAB computations with sparse and factored tensors. SIAM Journal on Scientic Computing, 30(1):205, 2008.

[3] J. Balani and L. Grasedyck. A projection method to solve linear systems in tensor format. Preprint 46 DFG-SPP 1324, Apr. 2010.

[4] W. Hackbusch and B. N. Khoromskij. Low-rank kronecker-product approximation to multi-dimensional nonlocal operators. part i. separable approximation of multi-variate function. Computing, 76(3-4):177{202, 2005.

[5] H. Kronmueller. Handbook of magnetism and advanced magnetic materials. J. Wiley & Sons, Hoboken New Jersey, 2007.

[6] I. V. Oseledets, D. V. Savostyanov, and E. E. Tyrtyshnikov. Linear algebra for tensor problems. Computing, 85(3):169{188, 2009

GUEST LECTURE: CLEMENS BECHINGER

Project Part	Date & Time	Presentation
GUEST LECTURE	Friday, 29.04.2011, 09:00 – 09:40	**"Colloidal Monolayers on Quasicrystalline Surfaces"** (35-40 min.)
	Clemens Bechinger *2. Physikalisches Institut, Stuttgart, Germany* *Monolayers on crystalline surfaces often form complex structures having physical and chemical properties strongly differing from those of their bulk phases. Such hetero-epitactic overlayers are currently used in nanotechnology and understanding their growth mechanism is important for the development of novel materials and devices. Compared to crystals, quasicrystalline surfaces exhibit much larger structural and chemical complexity leading e.g. to unusual frictional, catalytical or optical properties. Accordingly, deposition of thin films onto such substrates can lead to novel structures which may even exhibit typical quasicrystalline properties. Here we report a real-space investigation of the phase behaviour of a colloidal monolayer interacting with a quasicrystalline decagonal substrate created by interfering five laser beams. We observe a novel pseudomorphic phase which exhibits likewise crystalline and quasicrystalline structural properties. It can be described by an Archimedean-like tiling consisting of alternating rows of square and triangular tiles. In addition to establishing a link between Archimedean tilings and quasicrystals, our experiments allow to investigate in real space how single-element monolayers can form commensurate structures on quasicrystalline surfaces.*	

MEMO

GUEST LECTURE: SILKE BIERMANN

Project Part	Date & Time	Presentation
GUEST LECTURE	Thursday, 28.04.2011, 09:10 – 09:50	**"Strong Correlations from First Principles? A Dynamical Mean Field Viewpoint"** (35-40 min.)
	Describing strong electronic Coulomb correlations and their effect on the physical properties of materials is one of the bottlenecks of modern solid state physics. We will discuss this question from the dynamical mean field viewpoint, with transition metal oxides and pnictides serving as illustrations.	

MEMO

GUEST LECTURE: STEFAN MÜLLER

Project Part	Date & Time	Presentation
GUEST LECTURE	Friday, 29.04.2011, 09:40 – 10:20	**"Non-scalar Cluster Expansions for Arbitrary Configuration Dependent Observables"** (35-40 min.)
	Sascha B. Maisel, Nils Schindzielorz and Stefan Müller – Technische Universität Hamburg-Harburg, Institut für Keramische Hochleistungs-werkstoffe, Denickestr. 15, D-21073 Hamburg, e-mail: stefan.mueller@tuhh.de *Due to their predictive power, methods based on electronic structure theory are more and more applied for modelling real materials properties within a quantum mechanical framework. From a technical point of view, the vision behind is the design of functional materials with special properties before expensive experiments are performed. We use DFT-based approaches to calculate both free energies and various quantities of technological relevance for a giant number of atomic configurations. Of special interest are mechanical properties as elastic constants, bulk moduli or Zener ratio, and their relation to phase stability quantified by order parameters of high-end materials like Ni-rich alloys. Based on the formalism of the cluster expansion [1] as realized in the UNCLE [2] package, it is possible to expand any configuration dependent observable like the formation enthalpy in terms of its many-body interactions. In this talk, we present several cluster expansions performed for multiple observables simultaneously. These types of cluster expansion each yield the formation enthalpy plus one or more of the aforementioned other quantities. This enables us to relate e.g mechanical properties of a structure with its chemical stability. Supported by DFG.* *[1] J. M. Sanchez, F. Ducastelle, D. Gratias: Physica 128 A, 334, (1984).* *[2] D. Lerch, O. Wieckhorst, G. L. W. Hart, R. Forcade, S. Müller: Modelling Simul. Mater. Sci. Eng. 17, 055003, (2009).*	

MEMO

GUEST LECTURE: NICOLA SPALDIN

Project Part	Date & Time	Presentation
GUEST LECTURE	Thursday, 28.04.2011, 09:50 – 10:30	**"Computational Design of New Multifunctional Materials: From Magnetoelectronics to a Theory of Everything"** (35-40 min.)
	Nicola Spaldin – Department of Materials, ETH Zurich *As many talks in this workshop show, modern computational methods are proving to be invaluable in the first-principles design of new materials with specific targeted functionalities. I will illustrate their utility with two examples from the field of multiferroics: First, the design of new materials for electric-field control of magnetism, and second, testing extensions to the Standard Model by searching for the electric dipole moment of the electron.*	

MEMO

SCHEDULE

Thursday, 28. April 2011			
Time	**Title**	**Presenters**	**Details**
09:00 – 09:10	Greetings / Introduction	Georg Kresse	Greetings, Announcements
09:10 – 09:50	**"Strong Correlations from First Principles? A Dynamical Mean Field Viewpoint"**	Silke Biermann	Guest Lecture, 35-40 min., discussion included (5 min.)
09:50 – 10:30	**"Computational Design of New Multi-functional Materials: From Magneto-electronics to a Theory of Everything"**	Nicola Spaldin	Guest Lecture, 35-40 min., discussion included (5 min.)
10:30 – 11:00	Coffee Break (Buffet, Anteroom)		
11:00 – 12:00	**"Iron-based Superconductors from an LDA+DMFT Perspective"**	Markus Aichhorn	P03, 15-20 min. (11:00 – 11:20)
	"Dynamical Vertex Approximation for Nanoscopic Systems"	Angelo Valli	P03, 15-20 min. (11:20 – 11:40)
	"Wien2wannier: From Linearized Augmented Plane Waves to Maximally Localized Wannier Functions"	Philipp Wissgott	P03, 15-20 min. (11:40 – 12:00)
12:00 – 13:30	Lunch (Buffet, Anteroom)		
13:30 – 14:00	**"Self-consistent RPA Potential via the Sham Schlüter Equation"**	Georg Kresse	P02, 25-30 min., discussion included (5 min.)
14:00 – 14:30	**"Variational Optimization of the Numerical Renormalization Group"**	Iztok Pizorn	P04, 25-30 min., discussion included (5 min.)
14:30 – 15:00	**"Charge Exchange Between a LiF Surface and a Proton: An Embedded Cluster Approach"**	Franz P. Tiwald	P05, 25-30 min., discussion included (5 min.)
15:00 – 15:30	Coffee Break (Buffet, Anteroom)		
15:30 – 16:00	**"MCTDHF: state of the art"**	Norbert J. Mauser	P06, 25-30 min., discussion included (5 min.)
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Thursday, 28. April 2011			
Time	**Title**	**Presenters**	**Details**
16:00 – 16:30	**"Results of Advanced DFT Functionals with WIEN2k"**	Peter Blaha David Koller	P07, 25-30 min., discussion included (5 min.)
16:30 – 17:00	**"Magnetic Order in BaTiO3-xMx (M=C, N, B); the Search for Magnetic High Permittivity Materials."**	Christoph Gruber	P09, 25-30 min., discussion included (5 min.)
17:00 – 17:30	Location → General Meeting		
17:30 – 18:30	General Meeting (Room Nr. 55, Faculty of Physics, University of Vienna)		
18:30 – 19:00	Location → Restaurant ("Universitätsbräuhaus")		
19:00 – 21:00	Dinner (Buffet, "Universitätsbräuhaus")		
End of Day 1			

Friday, 29. April 2011			
Time	**Title**	**Presenters**	**Details**
09:00 – 09:40	**"Colloidal Monolayers on Quasicrystalline Surfaces"**	Clemens Bechinger	Guest Lecture, 35-40 min., discussion included (5 min.)
09:40 – 10:20	**"Non-scalar Cluster Expansions for Arbitrary Configuration Dependent Observables"**	Stefan Müller	Guest Lecture, 35-40 min., discussion included (5 min.)
10:20 – 10:50	Coffee Break (Buffet, Anteroom)		
10:50 – 11:20	**"First-principles Study of the $Fe_xNi_yAl_{1-x-y}$ Alloy System by the Cluster Expansion"**	Martin Leitner	P10, 25-30 min., discussion included (5 min.)
11:20 – 11:50	**"Analysis of the Influence of Vacancy-solute Interaction on Diffusion of Atomic Monomers and Clusters"**	Piotr Warczok	P10, 25-30 min., discussion included (5 min.)
11:50 – 12:10	Location → Restaurant ("Culinarium Cooking")		
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Friday, 29. April 2011			
Time	**Title**	**Presenters**	**Details**
12:10 – 13:20	Lunch (Buffet, "Culinarium Cooking")		
13:20 – 13:40	Restaurant ("Culinarium Cooking") → Location		
13:40 – 14:10	**"Self-Assembling DNA-coated Colloids. A Simulation Study"**	Panagiotis E. Theodorakis	P11, 25-30 min., discussion included (5 min.)
14:10 – 14:40	**"Stray Field Computation on Tensor Grids"**	Lukas Exl	P12, 25-30 min., discussion included (5 min.)
14:40 – 15:10	Coffee Break (Buffet, Anteroom)		
15:10 – 16:40	Discussion (Focus Groups, Location TBA)		
16:40 – 16:50	Farewell	Georg Kresse	Farewell, Announcements
End of Day 2, End of the Workshop			