KKR Workshop IV. Methodology and Applications

June 12-14, 2009

Research Institute For Solid State Physics and Optics, Hungarian Academy of Sciences, Budapest, Hungary

Sponsored by Psi-K, RISPO HAS, NEFIM

Organizers: B. Ujfalussy, L. Szunyogh, L. Udvardi, J. Kollar

Web page: http://kkrws.phy.bme.hu

The workshop was organized to continue the regular series of meetings of the Korringa-Kohn-Rostoker (KKR) research community under the support of Psi-K (Munich 2004, Bristol 2006, Canterbury 2008). The very purpose of the workshop was to keep the KKR method in the forefront of ab initio based computational materials science, by bringing together experts and students of leading groups in Europe, in the United States and in Japan. During the workshop, recent advances related to improved implementations of the KKR method, as well as it's applications to current problems of condensed matter science were discussed in detail.
Highlighted topics of the workshop were as follows:
(i) Methodological developments, with emphasis to large scale and full potential calculations. A special session focusing on these issues was devoted to the 60^{th} birthday of Rudi Zeller!
(ii) Functional materials for spintronics: oxides, half-metals and multiferroics.
(iii) Nanomagnetism and correlation effects in magnetic systems.
(iv) Finite temperature metallic magnetism in heterogeneous systems and nanostructured materials.

KKR-workshop, Budapest, June 12-14
Program

June 12, Friday

14:00 Welcome address (Laszlo Szunyogh, Balazs Ujfalussy)

Spintronics

14:05 Hisazumi Akai (Uni Osaka): New half-metallic antiferromagnets and their transport properties

14:30 Pawel Buczek (MPI Halle): Energies and life-times of magnons in half-metallic Heusler alloys

14:55 Dzidka Szotek (Daresbury): Structural phase transitions and fundamental band gaps $Mg_xZn_{1-x}O$ alloys from first principles

15:20 M. Carmen Muñoz (CSIC Madrid): Ferromagnetism at ZnO [0001] surfaces

15:45 Ingrid Mertig (MLU Halle): Ferroic materials and novel Functionalities

16:10-16:30 Coffee

Nanomagnetism, surface physics

16:30 Arthur Ernst (MPI Halle): Magnetism in nanostructures: first principles investigations with a multiple-scattering approach

16:55 Silvia Gallego (CSIC Madrid): Surface effects in the anisotropy of Co films

17:20 Jürgen Henk (MPI Halle): Rashba-type spin splitting in surface alloys

17:45 Samir Lounis (FZ Juelich): Observation of subsurface defects with the electron focusing effect

18:10 Phivos Mavropoulos (FZ Juelich): Lifetime Reduction of Surface States Caused by Impurity Scattering

June 13, Saturday

Correlated systems

9:00 Martin Lüders (Daresbury): The different flavors of SIC in DFT

9:25 Walter Temmermann (Daresbury): Disordered Local Moment Description of Magnetism in 3d-monoxides and heavy 4f ’s

9:50 S. Hossein Mirhosseini (MPI Halle): Self-interaction correction in Gadolinium: magnetic properties and surface states

10:15 Diemo Ködderitzsch (LMU Munich): Relativistic OEP for solids

10:40-11:00 Coffee

Spectroscopy

11:00 Jan Minar (LMU Munich): Correlation versus temperature: angle-resolved photoemission in the range between 10 eV and 10 keV

11:25 Ondrej Sipr (AS CR Prague): Role of valence-band correlations in XAS and XMCD spectra investigated via LDA+DMFT calculations

11:50 Masako Ogura (Uni Osaka): First-principles calculation of optical conductivity using the KKR-CPA method and Kubo-Greenwood formula

12:15 - 14:00 Lunch and Poster Session

Methodology, Full-Potential KKR

14:00 Rudi Zeller (FZ Juelich): Advances in the iterative solution of the TBKKR Dyson equation for large systems

14:25 Peter Weinberger (CNS Vienna): Describing surfaces: semi-infinite descriptions versus thin fim approaches

14:50 Hubert Ebert (LMU Munich): Solving the Poisson-equation within full-potential KKR calculations by means of Sacks's formula

15:15 Aurelian Rusanu & G. Malcolm Stocks (ORNL): Recent developments in Full-Potential MST at ORNL

15:40 Dmitry Fedorov (MLU Halle): Muffin-Tin Zero as a hidden parameter in the KKR method

16:05 Robert Hammerling (CMS Vienna): Magnetostatic energies in ab-initio magnetic anisotropy calculations

16:30 – 18:00 Coffee and Round-table Discussion

19:30 Banquet

June 14, Sunday

Magnetism

9:30 Balazs Gyorffy (Uni Bristol): KKR, Superconductivity and Magnetism

9:55 Sergeiy Mankovsky (LMU Munich): Exchange coupling tensor and its application to study magnetic properties of nanosystems using Monte Carlo simulation

10:20 David Bauer (FZ Juelich): Classical Spin Dynamics of Nanoclusters at Finite Temperature

10:45 Laszlo Udvardi (TU Budapest): Direct Monte-Carlo method for deposited magnetic nanostructures

11:10-11:30 Coffee

11:30 Laszlo Szunyogh (TU Budapest): Spin-Hamiltonian Based on the Relativistic Disordered Local Moment Scheme

11:55 Julie B. Staunton (Uni Warwick): The Relativistic Disordered Local Moment Theory of Magnetism: Magnetic Interactions in Heterostructures and Complex Lattices

12:20 Marcus Eisenbach (ORNL): Thermodynamics of magnetic systems from first principles: Combining Multiple Scattering ab initio methods (LSMS) with classical Monte-Carlo

12:45 Closing & lunch

Posters:

Stephan Lowitzer (LMU Munich): Calculating transport properties using the Kubo-Greenwood formalism

Corina Etz (MPI Halle): Ab–initio determination of the magneto–optical properties of $(Co_mIr_m)_n$ on Ir(111)

Martin Gradhand (MLU Halle): Calculation of relativistic wavefunctions in the KKR method

Steven Walczak (MLU Halle): Non-equilibrium Green's function approach in the KKR formalism

Guntram Fischer (MLU Halle): Calculation of Magnetic Properties in Correlated Systems

Alberto Marmodoro (Uni Warwick): Electrons in systems with several types and degrees of disorder: the Non-Local Coherent Potential Approximation for multi-atom per unit cell materials

Ivetta Slipukhina (CEA Grenoble): Magnetic properties and Mn-Mn exchange interaction in some intermetallic Mn-Ge compounds

Eszter Simon (RISPO Budapest): Anisotropic Rashba splitting and consequences on impurity interactions

Alexander Thiess (FZ Juelich): Massively Parallel Implementation of Lloyd's Formula

Manuel dos Santos Dias (Uni Warwick): Anisotropic Magnetic Correlations at Finite Temperature in RDLM

ABSTRACTS

New half-metallic antiferromagnets and their transport properties

H. Akai
Department of Physics, Osaka University, Japan

Half-metallic antiferromagnets are the materials that show no magnetization and yet half-metals. Such a property is important not only from a view point of basic physics but also from technological points of view. We have investigated a series of (AB)X2 (A, B=transition metal elements, X=S, Se, Te, N) intermetallic compounds of zincblende, NiAs, wurtzite, rock-salt, MnP and chalcopyrite type structures and have found that many of them become a half-metallic antiferromagnet. The electrical transport properties of TMR/GMR geometry composed of these half-metallic antiferromagnets were examined using KKR-CPA combined with Kubo-Greenwood formula. The results show that the systems are mostly stable in one of the above crystal structures and ideal as a pin-layer in TMR/GMR sensors.

Rashba-type spin splitting in surface alloys

J. Henk
Max Planck Institute of Microstructure Physics Weinberg 2, D-06120 Halle (Saale), Germany

In the emerging field of spintronics, numerous effects and proposed device applications rely on the Rashba effect in two-dimensional electron gases. A class of materials which shows an unmatched spin splitting are surface alloys which consist of heavy p elements (Pb, Bi) on fcc(111) metal surfaces (Cu, Ag). With our multiple-computer-code approach we have achieved a complete and consistent description of the spin-split surface states in these alloys. Using accurately determined surface geometries – obtained by VASP – the KKR code HUTSEPOT and the relativistic layer-KKR code *omni* provide detailed information on the spin-resolved electronic structure. On top of it, spin- and angle-resolved photoemission spectra computed with *omni* can be directly compared with their experimental counterparts. In the first part of my presentation, I am going to sketch our multi-code approach. In the second part, I will present typical features of selected systems: The unmatched spin splitting in Bi/Ag(111), the tunable Fermi energy in the disordered alloy Bi_xPb_{1-x}/Ag(111), and the unconventional spin topology in Bi/Cu(111).

Magnetism in nanostructures: first principles investigations with a multiple-scattering approach

A. Ernst
Max-Planck-Institut fur Mikrostrukturphysik, Weinberg2, D-06120 Halle, Germany

The multiple-scattering theory (MST) is an appropriate tool to describe electronic and magnetic properties of nanostructures. First, the MST provides explicitly the Green function, which is used in many applications of condensed matter physics. Second, the method can be easily formulated for any arrangement of atoms: from highly symmetrical structures to systems with absence of any kind of symmetry. Third, the MST can be efficiently optimized for the calculations of systems with a large amount of atoms. In my talk I shall present our recent investigations of electronic and magnetic properties of various nanosystems and heterostructures using a multiple-scattering approach implemented in the HUTSEPOT code1. In particular, I shall discuss spin waves in multilayered systems, the magnetism of iron islands on Cu(111), magnetic anisotropy of individual atoms and clusters of Fe and Co on Pt(111).

(1) The HUTSEPOT code is a common project of several institutions: MPI Halle, Daresbury Laboratory, the University of Bristol and the University of Warwick

Surface effects in the anisotropy of Co films

S. Gallego

Instituto de Ciencia de Materiales de Madrid, CSIC. Madrid, Spain

Ultrathin Co films on Ru(0001) form a unique structure which shows a variety of spin reorientation transitions depending on the number of Co atomic layers. Fully relativistic calculations based on the SKKR approach explain this surprising, rarely observed phenomena [1], where there is delicate competition between dipole, strain and stacking effects. Furthermore, the adsorption or capping of the surface with different elements has a determinant role in the easy magnetic axis, and depending on the element PMA (perpendicular magnetic anisotropy) may be either enhanced or destroyed [2,3].

[1] "Imaging spin reorientation transitions in consecutive atomic Co layers on Ru(0001)". F. El Gabaly *et al.*, Phys. Rev. Lett. 96, 147202 (2006).
[2] "Noble metal capping effects on the spin reorientation transitions of Co/Ru(0001)". F. El Gabaly *et al.*, New J. Phys. 10, 073024 (2008).
[3] "Band filling effects in the magnetic anisotropy of atomic thin layers of Co". S. Gallego *et al.*, Philos. Mag. 88, 2655 (2008).

Ferromagnetism at ZnO [0001] surfaces

M.C. Muñoz

Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid, Spain

Much effort has been devoted in the last decade to the search of room temperature ferromagnetism (RT-FM) in dilute magnetic oxides (DMO), particularly those based on ZnO. However, short ranged magnetic interactions and phase separation mechanisms seem to be major shortcuts for RT-FM in bulk DMO. Our first principles calculations of different low index ZnO surfaces indicate that

surface-induced p holes under excess Oxygen conditions lead to the formation of large magnetic moments even in the absence of magnetic dopants, the magnetic impurities serving to enhance the stability of these states [1]. Furthemore, the adsorption of atomic H at the Zn-ended (0001) surface induces spin-polarized states extending few atomic layers in depth and leading to a metallic surface. Hybridization enhances the strength of the magnetic interactions and gives rise to a ferromagnetic ground state [2].

[1] "Magnetic states at the Oxygen surfaces of ZnO and Co-doped ZnO". F. El Gabaly et al., Phys. Rev. Lett. 101, 067206 (2008).
[2] "H adsorption tunes ferromagnetism at the ZnO(0001) surface", N. Sanchez, S. Gallego, M.C. Muñoz (submitted to Phys. Rev. Lett.).

Advances in the iterative solution of the TBKKR Dyson equation for large systems

R. Zeller
IFF and IAS, Forschungszentrum Jülich GmbH, D-52425 Jülich

It is shown how the ideas of left and right preconditioning and iterative refinement can be applied for the iterative solution of the Dyson equation in the TBKKR Green function method. It is demonstrated that the combined use of these techniques leads to a reduction of the required number of iterations and thus to a considerable speedup of the calculations. It is discussed that these techniques do not prevent to obtain an algorithm with linear scaling computational complexity by a spatial truncation of the Green function.

Observation of subsurface defects with the electron focusing effect

S. Lounis
IFF Forschungszentrum Jülich GmbH, D-52425 Jülich, Germany

The Fermi surface that characterizes the electronic band structure of crystalline solids can be difficult to image experimentally in a way that reveals local variations. We show that Fermi surfaces can be imaged in real space with a low-temperature scanning tunneling microscope when subsurface point scatterers are present: in this case, cobalt impurities under a copper surface [1]. Even the very simple Fermi surface of copper causes strongly anisotropic propagation characteristics of bulk electrons that are confined in beamlike paths on the nanoscale. The induced charge density oscillations on the nearby surface can be used for mapping buried defects and interfaces and some of their properties.

[1] A. Weismann, M. Wenderoth, S. Lounis, P. Zahn, N. Quaas, R. G. Ulbrich, P. H. Dederichs, and S. Blügel, Science **323**, 1190 (2009).

First-principles calculation of optical conductivity using the KKR-CPA method and Kubo-Greenwood formula

M. Ogura
Department of Physics, Osaka University, Japan

The KKR-CPA method combined with the Kubo-Greenwood formula is one of the most powerful tools to calculate the transport properties. The formulation proposed by Butler is widely used in KKR or LMTO groups and has succeeded in explaining the electric conductivities of random systems. The technique to calculate the electric conductivity is easily expanded to the optical conductivity. In the present study, we present the calculation of the optical conductivity using the KKR-CPA method and Kubo-Greenwood formula. We propose a method to eliminate singularities which appear in conductivities and show the calculated results of optical conductivities including the MCD spectra of diluted magnetic semiconductors.

Magnetostatic energies in ab-initio magnetic anisotropy calculations

R. Hammerling
Wolfgang Pauli Institute and Center for Computational Materials Science Vienna, Austria

In this talk I will mathematically, critically review the ab-initio approach to Magnetic Anisotropy with focus on the description of magnetostatic energies. In particular thin magnetic films on surfaces will be presented. Magnetic anisotropy needs a Hamilton operator which (to some level) couples orbital and spin degrees of the electron. This can be realized coming from the nonrelativistic limit by adding certain terms to the Schrödinger operator or by using the Dirac operator coming from the relativistic side. The description of magnetostatic energies in ab-initio calculations at various levels (terms in Hamiltonian versus a-posteriori classical calculation) is reviewed. The different meaning of the term 'magnetization' between the ab-initio and micromagnetics approach is highlighted. Magnetostatic energies can be approximately calculated as sum over magnetic multipole moments. The inclusion of beyond dipole moments and intracell contributions is presented. Ab-initio results for $\ell > 1$ magnetic moments are given.

KKR, Superconductivity and Magnetism

B.L. Gyorffy
University of Bristol, UK

I will discuss the quasiparticle spectra of superconductor/ferromagnet multilayers with special reference to How and Why calculate it using the KKR method.

The Relativistic Disordered Local Moment Theory of Magnetism: Magnetic Interactions in Heterostructures and Complex Lattices.

Julie Staunton
University of Warwick, UK

We outline our ab-initio relativistic electronic structure theory for magnetic correlations and onset of magnetic order in complex materials. The theory is based on the Disordered Local Moment (DLM) description of magnetic fluctuations at finite temperatures as implemented through the Korringa-Kohn-Rostoker-Coherent-Potential-Approximation method. Since relativistic effects are fully incorporated the theory accounts for magnetic anisotropy. It describes the link between magnetic order and the spatial arrangement of the atoms of the material and does not require any fitting to an effective classical spin model Hamiltonian. We present preliminary results for Ir-Mn alloys.

Spin-Hamiltonian based on the Relativistic disordered Local Moment Scheme

L. Szunyogh
Budapest University of Technology and Economics, Budapest, Hungary

In order to derive tensorial exchange interactions and local magnetic anisotropies for itinerant magnetic systems in quite a general sense, a spin-cluster expansion is introduced as combined with the Relativistic Disordered Local Moment scheme. The theoretical background and the computational aspects of the method are discussed in details. First applications for ordered IrMn alloys as well as for a IrMn/Co interface are presented.

Thermodynamics of magnetic systems from first principles: Combining Multiple Scattering ab initio methods (LSMS) with classical Monte-Carlo

Markus Eisenbach
Oak-Ridge National Laboratory, Tennessee, USA

Density Functional Calculations have proven to be a useful tool to study the ground state of many materials. For finite temperatures the situation is less ideal an one is often forced to rely on models with parameters either fitted to first principles or experimental results. Here we describe a possible solution to this problem by combining the classical Wang-Landau method with our first principles multiple scattering code (LSMS). The combined code shows superb scaling behavior on massively parallel computers, having achieved 1.02 PFlops on the jaguar system at Oak Ridge. We show its ability to calculate magnetic phase transitions for bulk iron without the need to resort to external parameters.

Role of valence-band correlations in XAS and XMCD spectra investigated via LDA+DMFT calculations

Ondrej Sipr
Institute of Physics AS CR, Cukrovarnicka 10, CZ-162 53 Prague, Czech Republic
Universitat Munchen, Butenandtstr. 5-13, Germany

$L_{2,3}$-edge XAS and XMCD spectra of elemental Fe, Co, and Ni are calculated via a self-consistent LDA+DMFT method (inluding thus valence-band correlations). It is found that the asymetry of the calculated XAS white lines increases upon inclusion of the correlations for Fe and Co but not for Ni. The change in the height of the L_3 and L_2 peaks in the XMCD spectra is in a good agreement (verified by the XMCD sum rules) with the change of the orbital magnetic moment caused by adding the valence-band correlations. As a whole, adding valence-band correlations improves the agreement between the theory and experiment but visible differences still remain.

Magnetic properties and Mn-Mn exchange interaction in some intermetallic Mn-Ge compounds

I. SLIPUKHINA
Laboratoire de simulation atomistique (LSim), SP2M, INAC, CEA, 38054 Grenoble cedex 9, France

Mn-Ge intermetallic compounds exhibit a variety of magnetic properties, like ferro-, ferri-, antiferro- and parasitic ferromagnetism and can be considered as suitable candidates for their incorporation into spintronic devices. Here, we examine the ground-state and finite-temperature magnetic properties of the ferromagnetic Mn5Ge3 and MnGe2, as well as ferrimagnetic Mn5Ge2 compounds by means of first-principles calculations and Monte Carlo simulations. The ab initio electronic structure calculations are performed by the full-potential screened Korringa-Kohn-Rostocker (KKR) Green's function method. The exchange interaction parameters Jij are calculated using the Green's function formalism and the magnetic force theorem as implemented in the SPR-TB-KKR code [1]. The dependence of the exchange interaction and magnetic moments on the local environment and interatomic distances in different compounds is discussed. Based on the C-doped Mn5Ge3 compound as an example, the influence of the sp-elements doping on the Curie temperature in Mn-Ge system is considered and compared to the existing experimental data [2].

[1] The SPR-TB-KKR package, H. Ebert and R. Zeller,
`http://olymp.cup.uni-muenchen.de/ak/ebert/SPR-TB-KKR`
[2] I. Slipukhina, E. Arras, Ph. Mavropoulos, and P. Pochet, accepted for publication in Appl. Phys. Lett. (2009).

Calculation of relativistic wavefunctions in the KKR method

M. Gradhand
Martin-Luther Universität, Halle-Wittenberg, Germany

We want to present an implementation of wavefunction calculations in our relativistic KKR code. These wavefunctions are used to calculate spin expectation values on the Fermi surface of magnetic as well as non-magnetic materials. A description of spin-flip scattering time including the relativistic wavefunctions will be discussed.

Muffin-Tin Zero as a hidden parameter in the KKR method

D. Fedorov
Martin-Luther Universität, Halle-Wittenberg, Germany

I want to discuss the influence of a choice of muffin-tin zero value on results of electronic structure calculations. An idea of a "correct" choice for this parameter will be suggested. I will present a few examples of a practical implementaton of this idea.

Calculation of Magnetic Properties in Correlated Systems

G. Fischer
Martin-Luther Universität, Halle-Wittenberg, Germany

We present results of calculations of electronic and magnetic properties of different systems. These are the transition metal monoxides (MnO, FeO, CoO and NiO), defect-induced ZnO and the transition metal fluorides (MnF2, FeF2, CoF2 and NiF2). For the treatment of the localized d-electrons LSIC is applied. CPA is used to simulate the defects in ZnO. Magnetic interactions are mapped onto a Heisenberg Hamitonian by calculating the exchange parameters Jij via the Magnetic Force Theorem.

Electrons in systems with several types and degrees of disorder: the Non-Local Coherent Potential Approximation for multi-atom per unit cell materials" and short abstract: "We describe the extension of the KKR- non-local coherent potential approximation to materials with multi-atom per cell lattice structures. In such systems several ordering phenomena may be present and the disorder and development of SRO on one sub-lattice may be subtilely connected to properties associated with the atoms occupying another sub-lattice. We illustrate the extension of NLCPA method on a 1-d tight-binding model", to report on developments currently under preparation for publication.

Lifetime Reduction of Surface States Caused by Impurity Scattering

S. Heers
IFF Forschungszentrum Jülich GmbH, D-52425 Jülich

In order to describe the dynamics of charge transport, localization and quantum information on metal surfaces it is of crucial importance to understand the temporal evolution of quasiparticles (electrons and holes) in surface states, characterized by a lifetime τ. This lifetime is strongly reduced by scattering at impurities, vacancies and adatoms. Using the Korringa-Kohn-Rostoker Green function method [1], the elastic scattering rate $1/\tau$ can be calculated for adatoms as well as impurities and vacancies in and below the surface. We have performed calculations for the Cu (111) surface of finite-thickness slabs, investigating the lifetime of the Cu (111) surface state for the whole series of 3d transition metals as impurities. The thickness of the slab is varied, ranging from six to forty atomic layers. Our formalism allows us to separate the lifetime reduction induced by scattering to bulk states from scattering to surface states. We show that trends through the 3d series are qualitatively different for adatoms, compared to impurities in the surface. This work was supported by the ESF EUROCORES Programme SONS under contract N. ERAS-CT-2003-980409 and the Priority Programme SPP1153 of the DFG grand Bl 444/8-1.

[1] N. Papanikolaou, R. Zeller, P. H. Dederichs *J. Phys.: Condens. Matter* **14**, 2799 (2002).

Classical Spin Dynamics of Nanoclusters at Finite Temperature

David Bauer
IFF Forschungszentrum Jülich GmbH, D-52425 Jülich

Magnetic nanoparticles are promising candidates for future information storage. We developed a spin dynamics code and investigated the dynamics of the magnetization in nanoscale systems on the basis of a classical spin model including Heisenberg exchange, magnetic anisotropy, external magnetic fields and dipole-dipole interaction. The spin-system is coupled to a heatbath through a stochastic force within the Langevin approach [1]. This requires the solution of the stochastic Landau-Lifschitz equations. Thermodynamical properties are shown to be in excellent agreement to those obtained by Monte Carlo simulations. The complexity $\mathcal{O}(N^2)$ of the direct evaluation of the dipolar interaction was reduced to $\mathcal{O}(N \log N)$ by the use of multipole methods. Preliminary results are presented on the switching time of different sized nano-islands which are in agreement to the Arrhenius-Néel-law.

This work was supported by the ESF EUROCORES Programme SONS under contract N. ERAS-CT-2003-980409 and the Priority Programme SPP1153 of the DFG grant Bl 444/8-1.
[1] V. P. Antropov, S. V. Tretyakov, and B. N. Harmon, J. Appl. Phys. **81**, 3961 (1997).

List of Participants

Juergen Henk	Mpi-Halle	Malcolm Stocks	Oak Ridge
Guntram Fischer	Uni-Halle	Dmitry Fedorov	Uni-Halle
Pawel Buczek	Mpi-Halle	Martin Gradhand	Uni-Halle
Hossein Mirhosseini	Mpi-Halle	Robert Hammerling	Tu-wien
Alexander Thiess	Juelich	Masako Ogura	Osaka
Manuel dos Santos	Dias Warwick	David Bauer	Juelich
Alberto Marmodoro	Warwick	Samir Lounis	Juelich
Hubert Ebert	Munich	Peter Dederichs	Juelich
Diemo Kdderitzsch	Munich	Phivos Mavropoulos	Juelich
Steven Walczak	Uni-Halle	Corina Etz	Mpi-Halle
Stephan Lowitzer	Munich	Ivetta Slipukhina	Grenoble
Sergeiy Mankovsky	Munich	Ingrid Mertig	Uni-Halle
Jan Minar	Munich	Arthur Ernst	Mpi-Halle
M. Carmen Muoz	Madrid	Marcus Eisenbach	ORNL
Silvia Gallego	Madrid	Marcus Dane	ORNL
Julie Staunton	Warwick	Aurelian Rusanu	ORNL
Rudolf Zeller	Juelich	Eszter Simon	RISPO
Ondrej Sipr	AS CR	Janos Kollar	RISPO
Dzidka Szotek	Daresbury	Balazs Ujfalussy	RISPO
Walter Temmerman	Daresbury	Laszlo Szunyog	BME
Martin Lueders	Daresbury	Attila Szilva	BME
Balazs Gyorffy	Bristol	Laszlo Udvardi	BME
Peter Weinberger	Tu-wien	Laszlo Balog	BME
Hisazumi Akai	Osaka	Krisztian Palotas	BME