Periodic Progress and Final Report

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Foreword: Awards and Distinctions

Four nodes of our Network were honoured in the past year. Firstly, the experimental member Albert Fert from Orsay received the "2003 Medaille d'Or du CNRS" (Gold medal of the CNRS) for the discovery of the Giant Magneto-Resistance (GMR) and his contributions to the development of the field of magneto- or spinoelectronics. The CNRS-gold medal is extremely prestigious and only one medal is given each year for all fields of science. In 2004 Albert Fert was elected to the French Academy of Science.

Secondly, this Network in Computational Magnetoelectronics can be characterised by its research through strong networking. In particular I wish to highlight the Austrian-Hungarian-Czech collaboration which was selected as one of the 2004 finalists for the Descartes prize in the subject of Computational Science of Novel Materials.

Already in the beginning of the nineties close scientific relations between research groups in Budapest, Prague (Brno) and Vienna were established, devoted to electronic and magnetic properties of novel materials. The first common publications between Prague and Vienna appeared in 1991, those with Budapest a year earlier, since at that time the leader of the present Hungarian team was a PhD student in the Viennese research group. Since then not only a remarkable number of common publications appeared, but because of close interactions new theoretical approaches and computer codes were developed. These methods and codes are now widely used in the scientific community including for example such different places as the Institute des Solides, Université Paris Sud or the Nanostructure Center of Oak Ridge National Laboratory. It was in particular the interaction between different approaches and ideas that

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created a remarkable continental European intellectual atmosphere: by viewing problems from different angles and in communicating in colourful English.

Up to the very recent past the majority of activities was located at the Center of Computational Materials Science (CMS) in Vienna, now in Budapest as well as in Prague similar institutions exist. In the 4-th framework programme of the European Union the Czech and Hungarian scientists took part as “special guests” of the Austrian node, in the 5-th framework they already formed separate nodes, collaborating now partially via the present RT-network with the corresponding Austrian node. It is reassuring to see that independent of proposal calls or changes in national conditions the Austrian, Czech and Hungarian researchers continue to pursue a particular kind of research: computational science in novel materials. In this sense the Center of Computational Materials Science in Vienna added in a very special manner to the unification in Europe.

The “Computational Science of Novel Materials”-Team
Part A - Research Results

A.1 Periodic Progress Report: Scientific Highlights

Evidence for intrinsic ferromagnetism in Co-doped ZnO semiconductors

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A breakthrough in the field of new materials for spintronics was the report in 2001 of room temperature ferromagnetism in Co-doped ZnO films. Since then an intensive research has been carried out to assess the intrinsic nature of ferromagnetism in transition metal doped ZnO and rule out the presence of ferromagnetic transition metal clustering as an obvious origin of ferromagnetism. The CNRS-Orsay group of the French node has made significant progress towards this end in the last year of the network. Optimized Zn$_{0.75}$Co$_{0.25}$O thin films were grown by pulsed laser deposition on Al$_2$O$_3$(0001) substrates at 300°C under an oxygen partial pressure less than 10$^{-6}$ Torr. A detailed study of the local structural and magnetic properties of our films by X-ray diffraction, X-ray absorption spectroscopies (XANES, EXAFS, XMCD) and transmission electron microscopy was carried out. By combining these techniques no evidence of Co clustering was found which confirms the intrinsic nature of ferromagnetism in our Zn$_{0.75}$Co$_{0.25}$O films. A further confirmation came from the first experimental evidence of spin polarized tunneling of carriers in tunnel junctions of the type Zn$_{0.75}$Co$_{0.25}$O/Insulator/Co.

Although the results are promising, there is still a lack of understanding of the origin of ferromagnetism in this ferromagnetic semiconductor since the experimental Co magnetic moment per atom is significantly smaller than predicted by theory.

Magnetic Percolation in Diluted Magnetic Semiconductors

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Because of their ferromagnetism, the diluted magnetic semiconductors (DMS) represent a new class of materials with potential technological applications in the spintronics. The DMS with Curie temperatures of order of room temperature are needed for practical applications, whereas the currently prepared samples of Mn-doped GaAs exhibit Curie temperatures of about 170 K. Reliable determination of magnetic properties of DMS, in particular the critical temperature, is thus of great importance. By combining first principles calculations of interatomic exchange interactions with a classical Heisenberg model and Monte Carlo treatments of spin-fluctuations as well as the randomness of the underlying lattice, a theory that does not use any adjustable parameters was proposed. We have shown that the observed critical temperatures of a broad range of DMS, involving Mn-doped GaAs without and with As-antisites, Mn-doped GaN as well as Cr-doped ZnTe, are all reproduced with a good accuracy. An agreement between theory and experiment is obtained only when the magnetic atoms are randomly positioned on cation sublattices and when the chemical randomness and spin fluctuations are treated beyond the mean-field approximation. This suggests that the magnetic ordering temperature of diluted magnetic semiconductors is strongly influenced by magnetic percolation, which becomes more important for lower concentrations of magnetic impurities and for systems where the exchange interactions are strongly localized in the real space (Mn-doped GaN) (Phys. Rev. Lett. 93
Our analysis explains the wide interval of experimentally reported ordering temperatures, since the distribution of magnetic atoms on the cation sublattice is critically dependent on how the samples are prepared, resulting in a large range of ordering temperatures. In addition, the developed formalism represents a general scheme that can be applied to a number of other relevant problems in future, e.g., the effect of clustering of the magnetic atoms, the effect of electron correlations beyond the LSDA, the occurrence of magnetic atoms and defects on several sublattices, and many others.

Materials specific transport theory

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A tight-binding muffin-tin-orbital (TB-MTO) transport formalism was developed in Twente in which the scattering states are calculated explicitly, making it possible to perform "channel decomposition" of the scattering induced by specular interfaces, interface disorder etc. The calculation of the scattering matrices scales linearly with the number of principal layers \(L\) in the scattering region and as the cube of the number of atoms \(N\) in the lateral supercell. For metallic systems for which the required Brillouin zone sampling decreases as \(N\) increases, the final scaling goes as \(N^2L\). In practice, the efficient TB-MTO basis set allows scattering regions to be handled for which \(N^2L \sim 10^6\) and calculations have been carried out for lateral supercells containing 20x20 atoms in order to analyse the interface scattering at disordered Cu/Cu and Fe/Cr interfaces in an ongoing collaboration with the Delft node. The scheme has been used to study the influence of interface disorder on the giant magnetoresistance in both CPP and CIP geometries, on the spin-dependent interface resistance between the itinerant ferromagnet Fe and the prototypical semiconductor InAs, and on the suppression of Andreev reflection at interfaces between superconducting Pb and the transition metals Cu, Ni and Co.[PRL89, 166603 (2002); PRB65, 220401 (2002);PRB63, 064407 (2001)]

Transport and magnetic properties of M/X/M heterostructures (M=Fe, Co, or Ni, and X=Si, Ge, GaAs or ZnSe)

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The magnetic and transport properties of Fe(Co)Si/Fe(Co), Fe/Ge/Fe, Fe(Co)/GaAs/Fe(Co) and Fe/ZnSe/Fe trilayer heterostructures were studied by means of a Green’s function technique based on the tight-binding linear muffin-tin method. The interdiffusion at the interfaces is computed using the coherent potential approximation.

For all systems, we obtained a net charge transfer from the magnetic slab to the semiconducting region. The charge transfer, the magnetic moments of M atoms at the M/X interfaces as well as the exchange coupling between the magnetic slabs were found to be sensitive to the value of the lattice constant. In case of GaAs or ZnSe systems, the Fe and Co magnetic moments at the M/X interfaces depend of the terminations of the X semiconducting spacer, i. e., the Fe magnetic moment is higher for a Ga termination than for the As termination, and this difference results from a stronger hybridization between Fe and As atoms. We show that when the interdiffusion is confined to only two layers at the M/X interface the Fe(Co)/X(Fe(Co) (X=Si or Ge) interdiffused systems are unstable. To explain the stability of these systems a more sophisticated mechanism resulting in an extended alloy formation at the interface is required. For all systems in the ferromagnetic state, the majority-spin electron conductance is much larger than the spin minority one, and for both spin channels the conductance decreases rapidly to zero with
increasing spacer thickness. For the silicon systems, and for a small silicon thickness, negative values of tunnelling magnetoresistance ratio were obtained, in qualitative agreement with some experimental data. The strength of the conductance of the ferromagnetic state seems to be proportional to the sp density of states at the Fermi level, and the latter related to the strength of charge transfer at the M/X interface. Unfortunately, this proportionality does not hold for the the conductance of the antiferromagnetic state making the tunnelling magnetoreistance (TMR) hard to predict. Nonetheless the so called metal-induced gap states (MIGS) at the Fermi level which result from the hybridization of the metal states and the sp states of the semiconductor at the interface decrease exponentially in the barrier and might explain the trend of the TMR as a function of the semiconductor spacer. Thus, for the Si semiconducting spacer the MIGS decrease much slower than for systems with Ge or GaAs (ZnSe) spacers, resulting in a much higher value for the TMR ratio for this system.

**Electric transport through point contacts**

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Nanosized contacts between two macroscopic leads with single species (molecules, atoms) at its center attracted recently an intensive research interest. One of the most typical investigations are transport measurements showing, in particular, the by now well-known phenomena of conductance quantization and conductance fluctuations. Such systems are also possible candidates for spintronics devices. We employed a real-space formulation of the Kubo-Greenwood equation based on a Green's function embedding technique combined with the fully relativistic spin-polarized Korringa-Kohn-Rostoker method and performed a detailed investigation of the electrical transport through atomic-scaled contacts between two Au(001) semi-infinite systems. We studied the influence of transition metal impurities (Pd, Fe and Co) placed at various positions near the center of a particular contact and found that the conductance is very sensitive to the position of the magnetic impurities. The mechanism for the occurring relative changes can mainly be attributed to the impurities' minority d-band inducing resonant (Fano like) line-shapes in the s-like DOS at the center of the contact.

**Spin-transfer and magnetization-relaxation enhancement in thin magnetic films**

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The magnetization dynamics of small monodomain ferromagnets are well described by the Landau-Lifshitz-Gilbert (LLG) equation down to the micron scale. On the submicron scale, however, where the magnetization dynamics is no longer a highly coherent process because interfaces are relatively more important in small samples, new effects may play a role. One such effect, depending on the environment into which the ferromagnet is embedded, occurs when a time-dependent ferromagnetic order parameter pumps spin currents that carry angular momentum (and energy) into adjacent conducting materials. This angular-momentum loss is equivalent to a damping torque on the magnetization. It forms an additional, non-local source of ferromagnetic resonance (FMR) line broadening.

We used scattering matrices calculated from first-principles to study spin transfer and magnetization damping in layered systems comprising normal metal and ferromagnetic films. It was shown that the spin-current-induced magnetization torque is an interface effect and that quantum-interference effects are greatly overestimated by free-electron models and do not survive when realistic transition-metal band structures are used, especially when interface
The field of spintronics is concerned with search for highly spin-polarized materials for spin-dependent devices and spin-injection into semiconductors. Since true half-metals are extremely difficult to realize in practice, spin filtering can also be exploited to create near 100% spin polarization. The ferromagnetic insulating spinel transition metal oxides may very probably be used as tunnel barriers in spin-filtering devices. The filtering of electrons is dependent on the difference in the gap amplitude between the spin-up and spin-down channels of the barrier. Therefore it is of interest to use compounds for which this difference is greater and in this respect the electronic structure calculations could be of great help in providing guidance to experiments. To facilitate this we have studied the electronic structure of such spinel oxides as CoFe$_2$O$_4$ and NiFe$_2$O$_4$. The latter is known to be an inverse spinel system, with the octahedral sites occupied by the divalent Ni- and trivalent Fe-ions, and the tetrahedral sites by the trivalent Fe-ions. Using the first principles SIC-LSD-DFT approach we have concentrated on correlations between structure, valence and magnetism of these compounds and their influence on spin filtering properties. In particular, we have established that for NiFe$_2$O$_4$ the insulating inverse spinel structure is indeed the ground state, meaning that it is not energetically favourable to place 2+ ions on the tetrahedral sites, although in the normal spinel arrangement of ions, with the divalent Ni-ions on the tetrahedral sites, one observes a substantial increase both in the total spin moment (fourfold) and the spin splitting of the conduction band. This has been in line with recent experiments by A. Fert’s group in Paris that has seen a fourfold increase in the total magnetic moment of some thin film heterostructures of NiFe$_2$O$_4$. For CoFe$_2$O$_4$, a substantial increase in the conduction band splitting has also been calculated, together with more than twofold increase in the total spin moment, when changing from the inverse to normal spinel structure. However, the ground state in this case has been calculated to be a half-metallic, rather than insulating, state with all Fe- and Co- ions in the trivalent configuration. This finding does not necessarily exclude a possibility that the true ground state might be a mixture of the normal and inverse arrangements of ions, as some experiments might imply. In the normal spinel arrangement of ions, we have found both NiFe$_2$O$_4$ and CoFe$_2$O$_4$ to be just insulating, but possibly on the verge of becoming half-metallic.

Halfmetallic alloys are hybrids between metals and semiconductors: they show a metallic behaviour for electrons with one spin direction, usually for the majority electrons, but a semiconducting behaviour with a band gap at the Fermi level for the other (minority) electrons. Thus at the Fermi energy they exhibit a 100 % spin polarisation, which makes them prime candidates for applications in spintronics. In a series of articles the authors have investigated the fundamental electronic structure properties of such Heusler alloys, as well as the question, if
halfmetallicity, i.e. the band gap in the minority band, survives in real systems. The calculations for the ideal systems show, that (i) the band gap arises from the hybridisation between the d electrons of the magnetic transition metal atom and the non-magnetic one, (ii) the total magnetic moments $M_t$ follow a Slater Pauling rule $M_t = Z_t - 2N_o$ where $Z_t$ is the total number of valence electrons and $N_o$ the number of occupied minority bands ($N_o = 9$ for half Heusler alloys and $N_o = 12$ for full Heuslers). Relativistic calculations show that spin orbit coupling destroys the gap, at least in principle, but that in practice the spinpolarisation remains very high, say 99 %. In addition to the Heusler alloys we have also investigated the structurally similar halfmetallic zincblende compounds like CrAs. An important question is, if the halfmetallic behaviour prevails also at surfaces or at interfaces to semiconductors. The calculations show, that this is normally not the case, since localised dangling bond states appear in the band gap, similar to the behaviour observed at semiconductor surfaces. An exception are alloys containing Cr. Here the enhancement of the Cr local moment at the surface, the interface or in the multilayer can to a large extent preserve the gap, thus restoring the strong spin polarisation at $E_F$.

The authors are editing at present a book in the Springer series Lecture Notes on Physics with the title "Halfmetallic Alloys: Fundamentals and Applications". Furthermore I.G. has an invitation to write a review article for Reviews of Modern Physics.

**Half-Metallic Transition Metal Oxides**

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Due to the strongly correlated nature of their electrons, transition metal oxides are typically characterised by the coexistence of different kinds of order, including charge and orbital order, together with superconducting and magnetic order. Many of them are of interest for ‘spintronics’ applications due to their half-metallic characteristics. The 100 % spin polarisation at the Fermi energy makes them ideal materials for spin-dependent devices and spin injection. Using the SIC-LSD-DFT method we have studied the electronic and magnetic properties of magnetite and such half-metallic double perovskites as $\text{Ba}_2\text{FeMoO}_6$, $\text{Sr}_2\text{FeMoO}_6$, and $\text{Ca}_2\text{FeMoO}_6$. In magnetite, we have concentrated on the half-metal to insulator transition, associated with a lattice distortion from inverse spinel to monoclinic structure and charge order between trivalent and divalent Fe ions, induced on the octahedral sites. Exploring a number of charge order scenarios we have shown that a simple Verwey order is not the lowest energy solution, and the ionic picture is not valid. The calculated charge disproportionation of the half-metallic scenario, with all Fe ions in the trivalent configuration, has been found in good agreement with experiment, unlike that for the insulating Verwey phase, where trivalent and divalent Fe’s of the octahedral sites order in the alternating (001) planes. We have concluded that the structural distortions, more than localization/delocalisation correlations, are responsible for the charge disproportionation in the low temperature, monoclinic, phase of magnetite. In the double perovskites we have focussed on the Fe valence and the size and alignment of Fe and Mo spin moments to find contact with XMCD and NMR experiments. Based on the SIC-LSD-DFT calculations we have established that the half-metallic state in the studied double perovskites is driven by the interaction of the localized majority spin moment of the Fe$^{3+}$ ion and an itinerant minority electron with an induced spin moment composed of Fe and Mo $t_2g$ and oxygen 2p states. For all the perovskites studied, the calculated spin moments on Mo vary between -0.40 and -0.43 Bohr magnetons, and they are anti-parallel aligned with respect to Fe spin moments for all the compounds. This small variation has been confirmed by recent NMR experiments that have detected small differences in the Mo moments and they behave as we
have calculated them, namely in the Ca- and Ba-compounds the Mo moments are smaller than in the Sr-compound.

**Magnetic and transport properties of M/Cu/M multilayer systems (M=Fe, Co or Ni)**

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The magnetic properties of (semi-infinite Cu)/nM/mCu/nM/(semi-infinite Cu) (M=Fe, Co or Ni and n, m=integer number of M or Cu atomic monolayers) multilayer systems were studied by means of a Green’s function technique. The method is based on the tight-binding linear muffin-tin potential method in conjunction with the coherent potential approximation in order to describe the interdiffusion at the M/Cu interfaces. To calculate the transport properties in the ballistic limit in the current perpendicular-to-the plane geometry we used the Kubo-Landauer formalism. In case of Ni systems for smaller thickness of Ni magnetic slabs (n=1 or 2) no stable magnetic solutions were obtained. In case of Fe and Co systems at Fe(Co)/Cu interfaces there is a charge transfer from the magnetic slab to the non-magnetic Cu. At the M/Cu interfaces, there is an enhancement of the Fe magnetic moment while the Ni magnetic moment is reduced. The different magnetic behaviours of M atoms at the interfaces result from the competition between the narrowing of the density of states at the Fermi level due to the reduced coordination number and the decrease of the exchange splitting between majority- and minority-spin 3d sub-bands due to the hybridization between Cu and M states (sp-d and d-d). An oscillatory behaviour of the exchange coupling between ferromagnetic (FM) and antiferromagnetic (AFM) configurations with respect to the Cu spacer thickness was evidenced for all systems. The interlayer exchange coupling is influenced by the interdiffusion at the M/Cu interfaces. Thus in case of (semi-infinite Cu)/1Fe/3Cu/1Fe/(semi-infinite Cu) system a magnetic transition from the AFM to the FM state is obtained for the interdiffusion concentration c≈4% while for the (semi-infinite Cu)/1Co/3Cu/1Co/(semi-infinite Cu) the FM state remains more stable in the whole interdiffusion range. For (semi-infinite Cu)/3Ni/5Cu/3Ni/(semi-infinite Cu) system a transition from the FM to the AFM state was obtained for the interdiffusion concentration c=26%. For all systems in the FM states, the transmission amplitude of the majority-spin electrons is found to be much larger compared with the minority-spin ones. The oscillations of the giant magnetoresistance ratio are damped with increasing Cu spacer thickness. These oscillations originate from the oscillations of partial minority-spin conductance in the FM state.

**Anomalous magnetic anisotropy of Co monatomic wire at the Pt surface step edge**

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Recent progress in fabrication and characterization of the one-dimensional (1D) arrays of 3d metal wires at stepped Pt(111) surface made possible to observe, for the first time, the long-range magnetic order in 1D. Ferromagnetic order was demonstrated on Co wire decorating the Pt(997) surface step edge by Gambardella et al. (Nature (London) 416, 301 (2002)). Theoretically the Mermin-Wagner theorem (Phys. Rev. Lett. 17, 1133 (1966)) forbids long-range 1D ferromagnetic order at non-zero temperatures. Nonetheless, ferromagnetism in 1D can be stabilized by a large magnetic anisotropy energy, which creates barriers effectively blocking thermal fluctuations. We performed the first-principles calculations using the relativistic full-potential linearized-augmented-plane-wave (FP-LAPW) method, in which the spin-orbit coupling is included self-consistently using the second-variational procedure (Phys. Rev. B 56, R14259 (1997)). We used the so-called "magnetic force theorem" to compute the magnetic anisotropy energy (MAE). The key outcomes of our study (Phys. Rev. B 69, (2004)) are: an
easy axis at an odd angle rotated towards the Pt step edge, and an intrinsic noncollinearity between spin and orbital magnetic moments of the ferromagnetic Co wire and Pt substrate. We relate the origin of this novel magnetic behavior to the magnetic symmetry lowering at the surface step edge. We find a fair semi-quantitative agreement between our calculations and experimental data (Nature (London) 416, 301 (2002)): the calculated MAE difference between the hard and easy axes ~ 4.5 meV is somewhat bigger than experimentaly derived value of 2 meV/Co at T=45 K, and the calculated easy axis is rotated away from the z axis by the angle of 18 degrees which is smaller than the experimentally observed value of ~ 43 degrees. Our supercell model is a way too simple comparing with the measured system to expect a true quantitative agreement. For example the effect of structure relaxation near the step edge (not taken into account) can be very important. More realistic calculations are in progress.

Absence of zero-bias anomaly in spin-polarized vacuum tunneling in Co(0001)  
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One of the most striking effects in spin-dependent ballistic transport through planar tunnel junctions is the zero-bias anomaly (ZBA): the tunnel magneto-resistance (TMR) shows a pronounced maximum at zero bias voltage, in particular in junctions with oxide spacers. The origin of the ZBA was attributed to scattering at magnons and phonons as well as to scattering at defects while the density of states in the electrodes could be ruled.

In order to check the explanation by scattering at defects in the tunnel barrier, the oxide spacer was replaced by vacuum, thereby removing all scatterers from the spacer. Using a spin-resolved scanning tunneling microscope (Phys. Rev. Lett. 90 (2003) 116603), all other possible effects remain. Indeed, the experimental TMR for Co(0001) shows no ZBA, thus providing strong evidence for the defect hypothesis.

The experimental findings are fully supported by first-principles tunnel calculations within the Landauer-Büttiker theory as formulated in the layer-KKR method. Motivated by ab initio results for jellium, a heuristic potential within the vacuum region was introduced in order to treat a finite bias voltage (Phys. Rev. B 68 (2003) 174430). Superposing the image-charge potential between two metal surfaces and a linear potential drop with applied voltage, its shape is determined by the lead separation and the bias voltage. By this means, the absence of the ZBA in both theory and experiment is traced back to the electronic structure in the leads. Further, a distinct minimum in the experimental TMR at 0.2 eV bias voltage is explained by a majority surface state.

Surface-state electrons in atomic-scale nanostructures  
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Surface-state electrons on the close packed surfaces of noble metals form a two-dimensional (2D) nearly free electron gas. An electron in such a state runs along the surface, much like a 2D plane wave. The scattering of the surface-state electrons by adatoms leads to quantum-interference patterns in the local density of states (LDOS) [Phys. Rev. Lett. 90, 236801 (2003)] and to the long-range oscillatory interaction between adsorbates. These interactions were recently detected by STM and calculated by the ab initio method [Phys. Rev. B 68, 205410 (2003)] for separations of up to 70 Angstrom. It has been found that the long-range interactions can lead to an atomic self-assembly. In this way, new magnetic nanostructures with fascinating properties can be created [Phys. Rev. B 70, 075414 (2004)]. We have demonstrated that the controllable modification of the electronic confinement of surface-state electrons in atomically-engineered nanostructures, for example in quantum corals, could permit to manipulate the exchange interaction between magnetic adatoms at large distances [Phys. Rev. Lett. subm], and could be of a great importance for developing of quantum nano-devices.
Rashba-effect at (magnetic) metallic surfaces

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In semiconductor heterostructures, the Rashba effect allows the manipulation of spin-polarized electrons in a two-dimensional electron gas (2DEG) by an electric field. On metallic surfaces that support surface states, these surface states form a 2DEG that moves in the natural electric field provided by the surface. Using photoemission, the Rashba effect can be observed directly as spin-orbit splitting of surface states on some metal surfaces. This has been observed on Au(111) and H-covered W(110), but recently also on a number of Bi surfaces. Our ab-initio calculations clearly demonstrate that the surface states are indeed split by spin-orbit interaction [Phys. Rev. Lett. 93 46403 (2004)], and the effects can e.g. be seen analyzing quasiparticle interference patterns on a Bi(110) surface observed with STM [Phys. Rev. Lett. 93 196802 (2004)].

On magnetic metal surfaces, the 2DEG has additionally an exchange splitting that separates the spin-orbit split branches of the surface state. This allows an easier, spin-resolved observation of the Rashba effect as has been demonstrated for the first time on a magnetic surface, i.e. Gd(0001): In combination with first-principles calculations, this effect also opens up a new possibility to directly observe the magnetism of the surface layer and its modification by adsorbates (like O on Gd) on an atomic scale [Phys. Rev. Lett. submitted; cond-mat/0403405]. Comparing our calculations with experimental data, overall good agreement is found.

Spin-dependent scattering at semiconductor/ferromagnetic metal interfaces

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The holy-grail of “spintronics” is to combine the spin-degree of freedom so effectively used in metal-based magnetoelectronics (Giant MagnetoResistance effect), with the functionality and flexibility of semiconductor-based electronics. To do this requires being able to introduce and manipulate unpaired spins into semiconductors at room temperature. This remains a major challenge.

Attempts to realize this in a straightforward fashion by passing a current through an interface between a ferromagnetic metal and a semiconductor failed. This failure was explained in terms of the mismatch in the resistivities of metals and semiconductors: the large, spin-independent semiconductor resistivity completely swamps the small, spin-dependent ferromagnet resistivity. However, in this analysis, the interface resistance is neglected. By performing first-principles calculations for an Fe/InAs ohmic contact we showed that ideal interfaces have a spin-dependent resistance which is sufficiently large in absolute terms to make spin-injection possible. By performing calculations including disorder at the interface, it was also shown that the spin-dependence is very sensitive to such disorder. Similar calculations for Fe/GaAs Schottky barriers and for Fe/GaAs/Fe tunnel junctions confirmed this finding. [PRB 67, 092401 (2003)]

In addition to a majority-spin and a minority-spin interface conductance (or resistance), spin-transport through interfaces with ferromagnets are characterized by a complex-valued mixing conductance. The real part of the mixing conductance describes the angular momentum transfer to and from the ferromagnet, such as the strength of the spin-current induced magnetization torque or the non-local Gilbert damping. The imaginary part is an effective magnetic field.
These parameters can be expressed in terms of our microscopically determined scattering matrices. They were evaluated for the Fe/InAs interface and used to interpret recent experiments in which photoinduced carriers in a semiconductor were polarized by spin-dependent reflection.[PRL 92, 126601 (2004)]

**Magnetism in quantum corals**

Bence Lazarovits\(^1\), Balázs L. Györffy\(^{2,1}\), Balázs Újfalussy\(^{3,4}\), László Szunyogh\(^{1,5}\) and Peter Weinberger\(^1\)

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\(^5\)Budapest University of Technology and Economics, Budapest, Hungary

Over the past two decades, electrons in two-dimensional (2D) surface states on closed packed surfaces of noble metals have been at the center of much experimental and theoretical attention. For a pristine surface the energies of such states lay in the 'gap' around the L point of the bulk Brillouin Zone and the wavefunctions are confined to the surface. The most interesting feature of this remarkable state of matter is its response to perturbations such as caused by placing transition metal atoms on the surface. As might be expected, such response displays long range, 'Friedel like', charge oscillations governed by the 2D Fermi 'Surface'. Indeed, one of the iconic experiments in nano-technology has been the fabrication of a circular arrangement of 48 Fe atoms on a Cu(111) surface and the direct observation, by Scanning Tunneling Microscopy (STM), of such oscillations within the circle. We discussed the, as yet unexplored, spin-polarized properties of such quantum corals. We presented calculations for electronic and magnetic properties of surface states confined by a circular quantum corral built of magnetic adatoms (Fe) on a Cu(111) surface by showing the oscillations of charge and magnetization densities within the corral and the possibility of the appearance of spin-polarized states. In order to classify the peaks in the calculated density of states with orbital quantum numbers we analyzed the problem in terms of a simple quantum mechanical circular well model. This model is also used to estimate the behaviour of the magnetization and energy with respect to the radius of the circular corral.

**Ab initio spin dynamics approach to nanostructures**

Balázs Újfalussy\(^1,2\), Bence Lazarovits\(^3\), László Szunyogh\(^{3,4}\) and G. Malcolm Stocks\(^1\)

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\(^4\)Budapest University of Technology and Economics, Budapest, Hungary

Stimulated by the need for ever higher density recording media, atomic scale magnetic devices are presently at the very focus of experimental and theoretical research. Without doubt, understanding and design of the relevant physical properties - magnetic moments, magnetic anisotropy energies, thermal stability, switching - of atomic scaled magnets demand detailed knowledge of their electronic and magnetic structure. In order to search for the magnetic ground state of surface nanostructures we extended *first principles* adiabatic spin dynamics to the case of fully relativistic electron scattering. The method relies on a constrained density functional theory whereby the evolution of the orientations of the spin-moments results from a semi-classical Landau-Lifshitz equation. This approach is applied to a study of the ground state of a finite Co chain placed along a step edge of a Pt(111) surface. The ground state spin orientation tilted with respect to the surface normal is obtained in excellent agreement with the experiment. We also found that this magnetic state is *noncollinear*: a feature that is expected to play a key role in nanostructures having complex geometry.
A1 Final Report: Scientific Highlights

The previous 17 highlights together with the highlights of the previous three reports constitute a full record of all major achievements of this Network. Selecting only 5 highlights out of this would do injustice to all the fine achievements of this Network. In short, this Network has pioneered the application of ab-initio, materials specific calculations of both the electronic/magnetic and spin transport properties in materials of interest to spintronics. As such we have been extremely useful to the experimental work in this field, often guiding experimental searches for improved materials and properties.
A.2 Periodic Progress Report: Joint Publications and Patents


33) O. Eriksson, L. Bergqvist, B. Sanyal, J. Kudrnovský, V. Drchal, P. Korzhavyi, I. Turek, Electronic structure and magnetism of diluted magnetic semiconductors, J. Phys.: Condens. Matter (in print) SE-CZ collaboration

35) O. Šipr, M. Košuth, H. Ebert, Magnetic structure of free iron clusters compared to iron crystal surfaces, Phys. Rev. B 70 (2004) (in print), CZ-DEI collaboration


38) P. Vlaic, M. Alouani, O. Bengone, H. Dreyssé, Magnetism at the interface of M/S/M (M=Fe or Co; S=Si, Ge, GaAs or ZnSe), to be published, FR-SE collaboration.


**Single institute publications related to the contract.**


A2 Final Report: Joint Publications and Patents

The Network has published more than 250 joint publications (see the present report and the previous 3 reports). Inevitably there might be some double counting but this should not exceed more than 10%. Again selecting 5 publications would do injustice to all the fine work which was delivered by this Network. The Network comprised 10 scientific tasks each of which has led to numerous scientific publications.
Part B - Comparison with the Joint Programme of Work (Annex I of the contract)

B.1 Periodic Progress Report: Research Objectives

The research objectives, as described in Annex I of the contract, were all achieved. The Network's effort on the diluted magnetic semiconductors (DMS) continued vigorously and in particular the quest for room temperature ferromagnetism in DMS led to numerous studies of the finite temperature behaviour of the magnetic properties.

B.2 Periodic Progress Report: Research Method

The research methods as described in the contract have not changed. The strong activities in spin transport and correlations in novel magnetoelectronics materials characterised the Network. The methods used include the LDA+U and the self-interaction correction (SIC). In addition also more demanding methods like the GW approximation and the dynamical mean field approximation are being developed and are gradually applied to these materials.

B.3 Periodic Progress Report: Work Plan

Explain any significant differences in the current work plan in comparison to the original plan in the contract, in terms of:

- Breakdown of tasks
- Schedule and Milestones
- Research effort of the participants

No additional changes from the ones mentioned in the previous reports.
B.1 Final Report: Research achievements

Give an assessment of the research work actually carried out and the scientific results achieved in the course of the contract in comparison with the following aspects of the Joint Programme of Work:

- Research Objectives
- Research Method
- Breakdown of tasks
- Schedule and Milestones
- Research effort of the participants

The workplan has largely been implemented. Since the proposal was formulated the discovery of diluted magnetic semiconductors (DMS) occurred. The Network reacted on this admirably and its computational studies of DMS have made a major impact in the field. Hence, training was provided to young researchers working on 'hot topics'. Furthermore, the Network placed more emphasis on strongly correlated systems than originally planned. This was a consequence of the new materials for spintronics consisting of strongly correlated electrons.
B.4 Periodic Progress Report: Organisation and Management

B.4.1 The network's scientific tasks are organised into flagship projects and managed through a board of two to three of the most senior researchers in each node, coordinated through a Chairman and the Network coordinator. Open meetings of this board took place during the Network's annual meetings in Budapest (2001), Oleron (2002), Halle (2003) and St. Odile (2004), and also an exceptional meeting in Paris (2003). These meetings reviewed progress so far and in particular were instrumental in coordinating the training of the young researchers. The network uses the psi-k mailing list - which contains in excess of 1300 e-mail addresses of researchers active in ab initio electronic structure calculations to announce its meetings. Reports on these meetings are published in the psi-k newsletter which is distributed over the same mailing list. This newsletter is published every 2 months and available on the web (http://psi-k.dl.ac.uk). This web page also contains a pointer to the homepage of this RTN (http://psi-k.dl.ac.uk/index.html?magnetoelectronics).

B.4.2 Reports on Network Meetings
The Network organised in its fourth year three Network meetings which are reported below. The program of the meetings, the abstracts of all papers and the list of participants are published in the Psi-k Newsletter, which is available on http://psi-k.dl.ac.uk/index.html?newsletters. The respective issues of the newsletter are given below.

The third Annual Meeting of the RTN Computational Magnetoelectronics took place at the Max--Planck Institute in Halle, Germany, from Oct. 9--11, 2003. It was Organized by the Halle node, Wolfram Hergert in particular. The meeting was attended by 84 participants from 8 European countries. Every session started with an invited talk (1 hour), three of them (W. Kuch, Halle; K. Kern, Stuttgart and G. Seifert, Dresden) were experts outside the network. Members of the Network reported their results in 23 contributed talks (20 min each) and 34 poster presentations concerning the field of dilute magnetic semiconductors; surfaces, interfaces, nanostructures; oxides; transport properties; exchange interactions. There were very active discussions after each talks, but also during the poster session and the conference dinner. In a management meeting the future activities of the Network were discussed. More information: Psi-k Newsletter#60 (Dec. 2003).

This workshop was organized by Hubert Ebert from the University of Munich and Duane D. Johnson from the University of Illinois at Urbana-Champaign, USA from Febr. 13--15, 2004 at the University of Munich. The goal was to bring together European and US researchers developing and applying the Korringa--Kohn--Rostoker (KKR) electronic structure method, in particular to share recent advances and to enhance international collaborations on method and software development. The power and popularity of the KKR method arises from the fact that it gives directly access to the one-particle Green function and therefore allows applications to low dimensional systems, e.g. transport properties and to ab-initio many-body calculations. The workshop was attended by 54 participants which presented 23 oral and 24 poster contributions.

This workshop was organized by M. Alouani from the Strasbourg node in St. Odile near Strasbourg. It was motivated by recent advances in the treatment of electronic correlation effects, particularly in the context of realistic electronic structure calculations. The workshop attempted to balance two important components: (1) the development of new methods, and (2) applications of these methods to experimentally relevant systems, particularly in spintronics. A great progress in the field of strongly correlated electrons was made possible due to the new developments of both dynamical mean--field theory (DMFT) and the GW method combined
with realistic band--theory methods. This combined approach was central to this workshop. Thus, the realistic implementations of DMFT and GW constituted a great opportunity towards the solution of important problems which remained unsolved using traditional approaches. The workshop consisted of 23 invited presentations, mostly of 30 min each. All 40 participants agreed that the topic of the workshop will strongly affect the future research.

4. Other Workshop Activities of Network Members
Network Members played a leading role in many other activities outside the Network. For instance, the Halle node leader Patrick Bruno was the chairman of the 2004 Gordon Research Conference "Magnetic Nanostructures", Aug. 22--26, 2004, in Big Sky, Montana/USA. The Swedish Members Biplab Sanyal and Olle Eriksson organized a Summer School on "Magnetism and Transport in Solids", June 14--18, 2004 in Uppsala. Ingrid Mertig and Patrick Bruno organized a WE--Heraeus School "Physik magnetischer Nanostrukturen" in Halle, Sept. 13--24 2004. In all these schools, workshops and many other activities Network members were well represented and there were always invited speakers/lectures from our Network. Furthermore at the recent Nanospintronics Conference in Kyoto the list of invited speakers looked like a small Network meeting.

B.4.3 Networking
Describe the networking which has taken place during the reporting period, including for example secondments, short visits, bilateral meetings, e-discussions.

- Peter Dederichs (FZ-Juelich) visits Strasbourg node (IPCMS) and presents talk on "Dilute Magnetic Semiconductors"
- Peter Dederichs (FZ-Juelich) visits Vienna node and attends the Meeting of the International Advisory Board of the Institute for Computational Materials Science (CMS)
- Peter Dederichs, Samir Lounis, Phivos Mavropoulos and Rudi Zeller (FZ-Juelich) attend the KKR-Workshop in Munich, Febr. 20-22, 2004
- Peter Dederichs (FZ-Juelich) presents invited paper on "Spin Injection" at MRS-Meeting in San Francisco, April 12-16, 2004
- Stefan Bluegel, Peter Dederichs and Daniel Wortmann (FZ-Juelich) attend the International Conference on Nanospintronics in Kyoto, Japan, May 24-25, 2004
- Stefan Bluegel and Peter Dederichs (FZ-Juelich) attend the Gordon Research Conference "Magnetic Nanostructures" in Big Sky Resort, Montana, USA. Peter Dederichs presents an invited paper on "Exchange Interactions and Curie Temperatures in Dilute Magnetic Semiconductors"
- Stefan Bluegel, Peter Dederichs, Erik Koch and Rudi Zeller (FZ-Juelich) visit Workshop on Correlated Spintronics Materials in St. Odile (Strasbourg), Sept. 23-26, 2004
- I. Turek (CZ) visited O. Eriksson (S) (2-3 October 2003) to discuss future collaboration on diluted magnetic semiconductors and on transport in multilayers
- J. Kudrnovsky (CZ) visited P. Weinberger (A) (15 October - 15 December 2003) for a collaboration on exchange interactions in diluted magnetic semiconductors and spin glasses
- F. Maca (CZ) visited J. Redinger and P. Weinberger (A) (3-29 November 2003) for a collaboration on surface structure and magnetic anisotropy of thin film systems
- I. Abrikosov (S) visited J. Kudrnovsky and V. Drchal (CZ) (11-14 October 2003) in order to discuss various aspects of exchange interactions in random alloys
- O. Sipr (CZ) visited H. Ebert (D-1) (24-28 November 2003) to collaborate on magnetic structure of free Fe clusters
- V. Drchal (CZ) visited P. Weinberger (A) (6-11 November 2003) to complete a manuscript on phase stability of diluted magnetic semiconductors
- O. Eriksson (S) visited J. Kudrnovsky (CZ) (5-9 January 2004) for a discussion of results and preparation of a manuscript on magnetic percolation in diluted magnetic semiconductors
- V. Drchal (CZ) visited P. Weinberger (A) (March-May 2004) to collaborate on phase stability and electron correlation in diluted magnetic semiconductors
J. Kudrnovsky (CZ) visited S. Khmelevskyi and P. Mohn (A) (23-25 March 2004) to complete a manuscript on exchange interactions in spin glasses

J. Kudrnovsky (CZ) visited P. Bruno (D-2) (April-June 2004) to collaborate on diluted magnetic semiconductors, in particular to investigate the effect of electron correlations and to study their transport properties

O. Sipr (CZ) visited H. Ebert (D-1) (3-15 May 2004) in order to finish a manuscript on magnetic structure of Fe clusters and to discuss calculations of XMCD spectra of these systems

I. Turek and J. Kudrnovsky (CZ) visited P. Kelly (NL) (19 August 2004) to discuss a future collaboration on current-induced magnetization switching

I. Turek (CZ) visited S. Khmelevskyi and P. Mohn (A) (20-25 August 2004) for a discussion of magnetovolume phenomena in intermetallic compounds

I. Turek, J. Kudrnovsky, and V. Drchal (CZ) visited P. Weinberger (A) (13-14 September 2004) to discuss alternative approaches to current-induced magnetization reversal in multilayers

L. Sandratskii (D-2) visited J. Kudrnovsky and V. Drchal (CZ) (15-19 September 2004) in order to compare exchange interactions in magnetic semiconductors calculated by a frozen-magnon approach and a real-space technique

Stefan Bluegel (FZ-Juelich) gives lecture on "Rashba Effekt an Oberflächen" at WE-Heraeus School "Physik magnetischer Nanostrukturen" in Halle, Sept. 13-14, 2004. Peter Dederichs gives at the same School lecture on "Theorie des spinabhängigen Transports"

Stefan Bluegel (FZ-Juelich) gives lecture at the Summer School on "Magnetism and Transport in Solids", in Uppsala, June 14-18, 2004

Stefan Bluegel, Peter Dederichs (FZ-Juelich) and Ilja Turek (Brno), Josef Kudrnovsky (Prague) visit the Twente node of Paul Kelly and coworkers on Aug. 19, 2004 to discuss future collaborations.

F. Petroff of the F node gave a lecture at the summerschool on “New Magnetics” in Poznan (Poland), September 15-19, 2003

Seven members of the F-node attended the 3rd annual meeting in Halle (Germany), October 9-11, 2003.

N. Baadji student of the Strasbourg group of the F-node visited Prof. S. Bluegel (D-1, Juelich) from 15/01/04 to 15/03/04 January

O. Bengone from the SE node visited the Strasbourg group of the F-node, April 11-18, 2004

A. Fert of the F node gave a lecture at the “Swedish Summerschool on Magnetism and Transport in Solids” organized by the SE node in Uppsala (Sweden), June 14-18, 2004

Prof. J. Barnas (Poznan University) visited the CNRS-Orsay group of the F-node, June 22-25, 2004

Dr Dugaev (D-2 node) visited the CNRS-Orsay group of the F-node, June 21-26, 2004

Oct, 2003 László Szunyogh and László Udvardi attended third annual meeting of RTN in Halle, Germany

Feb, 2004 László Szunyogh, Balázs Újfalussy and László Udvardi visited MPI Halle (P. Bruno, I. Mertig)

Feb, 2004 László Szunyogh, Balázs Újfalussy and László Udvardi attended KKR workshop in München, Germany

Sep, 2004 László Szunyogh, Balázs Újfalussy and László Udvardi visited TU Wien (P. Weinberger)

Sep, 2004 János Kollár participates in a meeting in Brussels

Sep, 2004 Balázs Újfalussy visits Daresbury

Aug-Sep, 2004 Balázs Gyorffy is visiting expert in Budapest

P. Mohr (TU Wien) visited Uppsala University frequently.

H. Dreysse (Strassbourg) visited Uppsala University during autumn 2004.

J. Kudrnovsky (Prag) visited Uppsala University during spring 2004.

L. Bergqvist (Uppsala) visited Prag during autumn 2003.
- Peter Levy (US node) networks with Peter Weinberger (A) and Chuck Sommers (F).
- Walter Temmerman and Grzegorz Banach (UK node) attend the third annual meeting in Halle.
- Diemo Koedderitzsch attends a workshop in Aarhus Nov. 6-7, 2003.
- Walter Temmerman, Dzidka Szotek and Diemo Koedderitzsch attend the KKR workshop in Muenchen.
- Walter Temmerman and Dzidka Szotek give invited talks at the International Conference on Nanospintronics Design and Realization, Kyoto, Japan (May 24-28, 2004).
- Diemo Koedderitzsch perform a collaborative visit to Julie Staunton in Warwick.
- Dzidka Szotek and Walter Temmerman give talks at the workshop in St. Odile.
- Bagrets (Halle) visits the Dutch team (14/3 to 17/3/2003).
- Karas (Halle) visits the Juelich team (9/3 to 21/3/2003).
- Diemo Koedderitzsch and Wolfram Hergert (Halle) visit the Daresbury team (25/2 to 13/3/2003).
- Thirty participants of the Halle node at the third annual Network meeting.
- Seven participants of the Halle node at the Muenchen workshop.
- Visits of Ingrid Mertig (Halle) to Dusseldorf (17/3/2003) and Paris (24/01/2003).
- Summerschool on "New Magnetics" in Bedlewo 15 Sep 2003 - 19 Sep 2003 attended by: M. Zwierzycki (network postdoc).
B 2 Final Report: Overall Organisation and Management

The network's scientific tasks are organised into flagship projects and managed through a board of two to three of the most senior researchers in each node, coordinated through a Chairman and the Network coordinator. Open meetings of this board took place during the Network's annual meetings in Budapest (2001), Oleron (2002), Halle (2003) and St. Odile (2004). These meetings reviewed progress so far and in particular were concerned with the progress in the recruitment of young researchers.

The network uses the psi-k mailing list— which contains in excess of 1300 e-mail addresses of researchers active in ab initio electronic structure calculations to announce its meetings. Reports on these meetings are published in the psi-k newsletter which is distributed over the same mailing list. This newsletter is published every 2 months and available on the web (http://psi-k.dl.ac.uk). This web page also contains a pointer to the homepage of this RTN.

Communication strategy
Most of the communication took place electronically via e-mail. This was sometimes augmented with Access Grid conferences between Juelich and Daresbury. The latter would become the preferred communication medium is available with all the teams. However, the annual remained indispensable for the smooth running of the Network. This was the only time researchers, young and old alike, has enough time for in-depth planning of future activities.

Dissemination of Network's achievements
• Psi-k Newsletter, distributed electronically to 1,300 addresses, included abstracts of submitted papers, announcements of workshops and detailed reports on all Network activities (with program, abstracts and list of participants).
• The Network members and the results of their work were present at all major conferences and workshops in the field. There was hardly an international conference, where Network members were not invited as speakers. At some conferences, in particular at the Nanospintronics Conference in Kyoto in 2004, the list of invited speakers looked like a small Network meeting.
• Network members were very active in many other conferences and meetings outside the Network. Some examples are:
  o Gordon Research Conference "Magnetic Nanostructures" in Il Ciocco, May 12-17, 2002, Vice chairman Patrick Bruno (Halle)
  o 3 Minicolloquia at EPS-CMD19 Conference in Brighton, April 7-11, 2002 were organised by Network members
  o Several satellite Workshops at BESSY User Meetings were organised by Paul Strange (Keele) and Hubert Ebert (Munich)
  o Gordon Research Conference "Magnetic Nanostructures" in Big Sky, Montana (2004), Chairman Patrick Bruno (Halle), (Stefan Blügel elected as Vicechair for next conference in 2006)
  o Swedish Summerschool of "Magnetism and Transport in Solids", June 14-18, 2004; Organisers Biplab Sunyal and Olle Eriksson (Uppsala)
  o WE-Heraeus School "Physik magnetischer Nanostrukturen" in Halle, Sept. 13-24, 2004; Organisers Ingrid Mertig and Patrik Bruno
  o WE-Heraeus Seminars at Bad Honnef were organised by Stefan Blügel (2003) and Hubert Ebert (2002)
  o IFF-Spring School "Magnetism goes Nano", Research Center Juelich, Feb. 2005 with 270 registered participants, Coorganiser Stefan Blügel

List of Network Meetings
1) RTN Workshop on TMR and GMR in Dresden, Dec. 1–3, 2001
   54 participants Report in: Psi-k Newsletter #43 (Febr. 2001)
   113 young researchers, 29 lectures Psi-k Newsletter #46 (Aug. 2001)
3) 1st Annual Meeting in Budapest, Sept. 27-20, 2001
77 participants  
 Psi-k Newsletter #49 (Feb. 2002)

4) Hands-on KKR and Spectroscopics Course in Munich, Feb. 19-22, 2002  
32 young researchers, 14 lectures/tutors  
 Psi-k Newsletter #51 (June 2002)

5) RTN Mini-Workshop "Novel Magnetoelectronics Materials" at Orsay, Feb. 8, 2002  
25 participants  
 Psi-k Newsletter #50 (April 2002)

6) Swedish Summerschool on "Magnetism", in Backagarden, Sweden, July 1-5, 2002  
50 young researchers, 18 lectures  
 Psi-k Newsletter #53 (Oct 2002)

7) 2nd Annual Meeting and Midterm Review on Oleron (France); Oct. 5-9, 2002  
80 participants  
 Psi-k Newsletter #54 (Dec. 2002)

19 participants  
 Psi-k Newsletter #55 (Feb. 2003)

63 participants  
 Psi-k Newsletter #57 (June 2003)

10) Workshop on "Diluted Magnetic Semiconductors" at CECAM, Lyon, June 12-14, 2003  
52 participants  
 Psi-k Newsletter #58 (Aug. 2003)

61 participants  
 Psi-k Newsletter #59 (Oct. 2003)

12) 3rd Annual Meeting in Halle, Oct. 9-11, 2003  
84 participants  
 Psi-k Newsletter #60 (Dec. 2003)

13) KKR-Workshop: New Developments, Applications and Collaborations, Munich,  
Feb. 13-14, 2004  
54 participants  
 Psi-k Newsletter #62 (Apr. 2004)

14) Workshop on ab-initio Methods for Correlated Spintronics Materials and 4th Annual  
Meeting, Strasbourg, Sept. 23-26, 2004  
40 participants  
 Psi-k Newsletter #67 (Feb. 2005)

**Total No. of participants at Network meetings: 865**

**Networking activities:**

In short, the networking activities consisted of:

1) 14 Network conferences with in total 865 participants
2) about 250 joint publications
3) substantial amount of secondments, exchange visits, etc (for the 4th year more than 60 are listed in B4.3)
4) 307 person months of training

This speaks for itself: In the field “Computational Magneto-electronics” the Network has done a magnificent job both in training and in research. Moreover, it has achieved a lasting unification of Europe in this field.
B.5 Periodic Progress Report: Training

B.5.1 Describe the measures taken to publicise vacant positions. The psi-k mailing list has been used to advertise the vacant positions.

B.5.2 Using the table shown below, compare the progress in recruitment of young researchers (Pre-Doc and Post-Doc) with the plan in the contract. (Note that columns a and b must be identical to the figures laid down in Annex I of the contract). Comment on the progress of recruitment to date. All the nodes, bar D-2 and NL, have delivered more training months than promised in the contract.

<table>
<thead>
<tr>
<th>Participant</th>
<th>Contract deliverable of Young Researchers to be financed by the contract (person-months)</th>
<th>Young Researchers financed by the contract so far (person-months)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Pre-doc (a)</td>
<td>Post-doc (b)</td>
</tr>
<tr>
<td>UK</td>
<td>57</td>
<td>57</td>
</tr>
<tr>
<td>D-1</td>
<td>26</td>
<td>26</td>
</tr>
<tr>
<td>D-2</td>
<td>33</td>
<td>33</td>
</tr>
<tr>
<td>F</td>
<td>46</td>
<td>46</td>
</tr>
<tr>
<td>A</td>
<td>36</td>
<td>36</td>
</tr>
<tr>
<td>NL</td>
<td>28</td>
<td>28</td>
</tr>
<tr>
<td>S</td>
<td>33</td>
<td>33</td>
</tr>
<tr>
<td>TOTAL</td>
<td>259</td>
<td>259</td>
</tr>
</tbody>
</table>

In total the Network has delivered nearly 20% more training months than requested by the contract.

B.5.3 Describe how the young researchers have been integrated into the research programme. Attendance at the 3 Network Meetings (see B.4.2).

B.5.4 Describe the special measures being undertaken to train the young researchers, in particular training through visits and secondments, training on specialised instruments, presentations at conferences etc. Explain any differences in comparison to the contract. All young researchers attended the annual meetings.

B.5.5 Describe the special measures if any, which have been taken to promote equal opportunities.

B.5.6 If relevant, describe the measures being taken to exploit multidisciplinarity in the training programme.
B.5.7 If relevant, describe how connections to industrial and commercial enterprises have been exploited in the training programme.
B3 Final Report: Training Overview
The young researchers were recruited mostly through the Psi-k network and they found employment afterwards through the same network. There were problems recruiting young researchers of the right calibre. Especially the Halle node encountered severe problems which were mostly due to location. Therefore the Network produced many more pre-doc training months than originally anticipated. These pre-doc researchers turned out be very beneficial for the Network. Of course for the big laboratories it is much more difficult to employ these pre-doc researchers than for the Universities who can deliver Ph.D. degrees.

B 4 Final Report: Industry Connections
The Industrial partner changed from Thomson to Thales and the French node is now associated with this firm. A firm collaboration between Thales and the Swedish, British and American nodes have developed in the area of novel magnetoelectronic materials and current driven magnetisation switching. Moreover Thales organised the Mini-Workshop "Novel Magnetoelectronics Materials" (at Orsay on Febr. 8, 2002) which was particularly devoted to interaction between the theory groups and the experimental Thales group.

B5 Final Report: Recommendations
We enjoyed the collaborating in this Network and having the opportunity to train young researchers. These researchers have been able to contribute at the frontiers of science and that was very rewarding for all involved. This is the bit enjoyed by all. The negative aspects are all the restrictions imposed on how the monies are to be divided. One node had problems recruiting and this had a knock-on effect on all the nodes because of the 60-40 rule. This problem was exacerbated due to the fact that the Network had two nodes (CZ and HU) which received only travel expenses. When trying to deal with this through an extension of the Network, this was dealt with very unsympathetically by the Brussels bureaucrats. In short, there is a big gap between the good intentions as formulated in the rules and the reality on the ground and this is exacerbated by the inflexibility of the bureaucracy.
B.6 Periodic Progress Report: Difficulties

The Network applied for one year's extension without additional funding. This was refused. The reasons for the application were, firstly, to give the Halle node an additional year to deliver its promised training months and to reduce its budget underspend of 67%. Secondly, to ensure that 60% of the budget was spent on the young researchers. In the final cost statements 59.6% was spent on young researchers and we hope that the Commission will find this adequate given that the extension requested to redress this was refused and that the Network had two nodes with travel expenses only. In the end the Network spend 94% of its budget with the following nodes underspending: UK (3%), Halle (67%), Austria (9%), Hungary (8%), Czech Republic (2%) and the following nodes overspending: Juelich (3%), France (13%), Netherlands (7%), Sweden (23%).