Research Networking Programmes

Science Meeting – Scientific Report

***Proposal Title*: Computation meets Experiment: KKR Greens functions for calculations of spectroscopic, transport and magnetic properties**

Application Reference N°: 4608

1) Summary

Details about the meeting can be found at
http://www2.warwick.ac.uk/fac/sci/physics/events/kkr_greens/

Density-functional theory (DFT) calculations form a key research methodology in materials science. Calculations of many properties can be compared to experiment and guide the development of simpler phenomenological models. In this context codes built around the computation of the Kohn-Sham Green Function, in particular those based on the KKR method, give immediate access to spectroscopic properties and provide the ideal components for evaluation of transport and response functions and so on. Such codes are especially useful for the study of electron systems with narrow electron bands of d- or f-like character, associated with transition metal or rare earth atoms. A host of important new physical phenomena occur when such narrow bands lie near the Fermi level. Experimental study of these materials is one of the largest and most important areas of condensed matter physics, in which major investments have been made in experimental facilities world-wide. This 3-day workshop "Computation meets experiment: KKR Green functions for calculations of spectroscopic, transport and magnetic properties" sought to bring together experimentalists whose observations and analysis might stimulate and benefit from the work of theoreticians in the electronic structure DFT community who use Green's function and related methods. The workshop followed a 4-day CECAM-funded, hands-on tutorial on the SPR-KKR computational code for 29 students and preceded an EPSRC funded session, dedicated to creating new common projects between different communities.

2) Description of the scientific content of and discussions at the event

The workshop program was split into 7 sessions, with invited talks (25 min. + 5 min. discussions) and contributed talks (20+5 min.). All sessions were devoted to particular subjects combining invited talks from experimental colleagues with corresponding theoretical contributions. At the end of each session there was an additional 15 minute slot which was used to prompt discussions about general experimental and theoretical trends in a given topic. These periods were important parts of the workshop - the discussions were lively and gave clear indications about what theoretical developments are needed to help the understanding of certain experimental findings. They also showed what additional experiments might help theoreticians to check and assess their computational codes, approximations used and methodological accuracy.

The first two sessions of this workshop were devoted to the field of electronic spectroscopies. Spectroscopy is an extremely important experimental tool providing information about the electronic structure of the probed system and as such is a stringent test for any electronic structure theory. The presentation of N. Plumb showed a clear demonstration that the combination of modern experimental techniques like angle-resolved photoemission (ARPES) and resonant inelastic scattering (RIXS) are necessary to understand electronic properties of complex oxides. In addition G. Parakhonskiy discussed recent X-ray absorption measurements (XAS) of 3d melts under high pressures. The use of a multiple scattering Green's function framework results in a very flexible and accurate description of these spectroscopic techniques. This was demonstrated by two talks by M. Lindroos and J. Braun where they discussed new theoretical developments in the implementation of the one step model of ARPES. Illustrations of the benefits of employing this method were the prediction of ARPES spectra of topological insulators (J. Braun) and high temperature superconductors (M. Lindroos). On the other hand, the description of resonant processes such as RIXS and resonant photoemission (RPES), still needs to be developed within the KKR method. First steps towards this direction were shown by J. Rehr (RIXS) and P. Krueger (RPES).

Application of the standard experimental electronic spectroscopies mentioned above to hybrid systems (e.g. magnetic organic complexes deposited on transition metal surfaces) was presented in two experimental talks (F. Reinert and H. Wende). H. Wende showed by means of the observed magnetic circular dichroism in XAS that these materials show very interesting magnetic properties that may be used in spintronic applications. Owing to reduced dimensionality exotic correlation effects such as the Kondo effect can be observed in these hybrid materials (F. Reinert). Intensive discussions between experimentalists and theoreticians gave clear hints for further developments of KKR Green's function methods that will be required to produce a realistic theoretical description of these organo-metallic systems.

Scattering-based techniques give access to equilibrium properties of magnetic materials. J. Duffy highlighted the application of magnetic Compton scattering for the determination of the spin-polarised electron momentum density and consequently Fermi level spin polarisation of ferromagnetic materials. Such information is important for the development of novel spintronic materials. S. Dugdale showed how the closely related 2D-ACAR positron annihilation technique gives direct access to the Fermi surface morphology via the electron-positron momentum density. Both talks showed also how necessary it is to interpret experimental data by using theoretical methods, e.g. KKR. On the other hand it was also clearly shown that developments of the methods beyond standard LSDA are necessary to describe experimental data for many rare earth and transition metal magnetic materials.

Several sessions were devoted to the broad field of magnetism which is the domain of many modern applications of the KKR. The talk by C. Marrows addressed the new field of Skyrmions, magnetic twisted vortex structures stabilized by the Dzyaloshinsky-Moriya exchange interaction. These structures are candidates for new spintronic storage elements with the advantage that they need extremely small current densities to switch. He gave experimental evidence for the existence of Skyrmions in Co-doped FeSi epilayers and further possible experimental verification via, for example, transport measurements was discussed. An important property of a magnetic system is its magnetic phase diagram. This was subject of the talk by L. Szunyogh who introduced the implementation of a relativistic disordered local moment (R-DLM) method within the KKR and how it describes the dependence of the magnetic state of a metal on temperature and/or applied magnetic field. Magnetic excitations are an important aspect when studying the dynamics of the magnetization processes that are relevant for storage technologies. K. Zakeri discussed the role of spin-orbit coupling during the excitation process in ultrathin magnetic films. H. Ebert addressed the issue of the magnetic damping in ferromagnetic metals and alloys that is directly related to the spin-coupling in these systems. These damping processes are described by a classical Landau-Lifshitz-Gilbert equation. Its damping parameters have recently become accessible from *ab-intio* quantum mechanical calculations using a linear response KKR-framework. S. Lounis showed an alternative approach based of the combination of time dependent density functional theory and KKR to describe spin fluctuations in small clusters deposited on the surfaces. Ensuing discussions after the talks between experimentalists and theoreticians gave important directions for extending these studies.

Another important aspect was “materials design” and featured in several experimental as well as theoretical talks. G. Balakrishnan addressed the synthesis and study of Topological Insulators (TOPOs), a new class of matter insulating in the bulk but metallic at the surface. These materials have been recently predicted by theory and subsequently experimentally identified. At the moment these systems are being intensively studied and their potential for spintronics applications is clearly recognized. With the lack of a fully unambiguous experimental evidence of the topological state, it is of paramount importance to search for materials displaying this property in reproducible experiments aided by first-principles computations. This has already been started by coupling spectroscopies with first-principles KKR computations. A talk by J. Honolka on X-ray absorption spectroscopy of magnetic atoms coupled to topological insulators addressed this issue directly. Further experimental talks by D. Paudyal and E. Blackburn presented results on rare earth based materials and the HTC cuprates. A theoretical talk given by A. Ernst addressed the first-principles design of complex oxides. Strongly correlated transition-metal oxides are unsatisfactorily described within the local density approximation of density-functional theory. This talk and ensuing discussions demonstrated that by including suitable corrections, i.e. self-interaction corrections (SIC) or LSDA+*U*, design of complex systems is possible. Nonetheless the consensus is that these are only intermediate steps towards more systematic approaches. The electronic structure of all the mentioned systems – topological insulators, cuprates, rare earth systems and complex oxides – is accessible with the all electron KKR-GF method demonstrating its versatility. Whereas the last three classes have been studied in detail over several years, the study of topological insulators by means of the KKR-GF method is in its early stages. It became clear from the meeting that the KKR-GF will be able to treat a wide range of aspects of the TOPOs, i.e. the electronic structure, transport, disorder, spectroscopy, etc. in a consistent manner.

Several talks were devoted to the study of electronic transport. The former subject of TOPOs was also addressed in an experimental talk on transport in these systems by S. Fischer who presented combined structural, electronic and transport investigations of the undoped topological insulator Bi_2Se_3. At the moment transport in TOPOs is only dealt with on a simple model level for a few case studies. First-principles descriptions are still lacking. Given the huge promise of these systems in spintronics applications it is important to have a first-principles level description of their transport. Systems that have topological aspects in common with the TOPOs are materials in which the so called spin Hall effect, resulting from spin-orbit coupling, is operational. This effect has indeed been described within KKR-GF based transport frameworks, i.e. the Boltzmann approach and the Kubo formalism. Therefore, the description of transport in TOPOs within KKR-GF looks readily feasible. This was the conclusion of discussions after the presentations. The talk by M. Gradhand presented results on Hall effects in unconventional superconductors hinting at the bridge to the TOPOs. P. Mavropoulos in his talk presented KKR-GF calculations on the spin-relaxation time in metals. A further effect with application in spintronics, the tunneling anisotropic magnetoresistance (TAMR), was discussed in theoretical talks by J. Zemen and I. Turek.

Several talks addressed new developments within the KKR-GF framework to advance the method and to respond to challenges posed by experiment. Whereas transport calculations including a bias employing a non-equilibrium Green-function method are tackled in many studies on a model level, ab-initio based descriptions have only recently been developed. Still many technical problems and fundamental issues remain to be overcome. Two talks were devoted to this particular subject: H. Akai presented his implementation of the non-equilibrium GF method and gave useful pointers to help other code developers deciding to pick up this approach. Ch. Heiliger also presented an implementation of the non-equilibrium GF method. In particular he outlined his recent developments to include the so called vertex corrections. Application to magnetic alloy tunnel junctions impressively showed the heavy impact of vertex corrections but also highlighted that several problems have to be solved to moderate the massive computational effort when using this approach for large systems. In a talk by R. Zeller two main issues were addressed: a vision where the KKR-GF method is fully exploiting multicore grid architectures and a solution to the long standing issues of the KKR-GF angular momentum (l) convergence. Finally, M. Däne presented a new self-interaction correction approach that, as seen above, is one direction within DFT to address the problems of the description of strongly correlated systems (see also above “materials design”).

A poster session complemented the event by allowing participants to continue discussions and, in particular, to initiate new collaborations between experimentalists and people from the KKR community. In passing we should mention the importance of all the informal discussions that were carried over to the dinner and lunch breaks which the Warwick University Campus venue facilitated. The venue assembled and accommodated the participants on one self-contained site which meant that there were plenty of other chances to extend discussions in various locations (coffee lounges/bars).

3) Assessment of the results and impact of the event on the future directions of the field

In assessing the general outcome of the workshop we can state that indeed computation successfully met experiment, insofar as lots of discussions between scientists from the KKR community and experimentalists took place that gave important hints for future directions in program development. Also, the experimentalists obtained insight into state of the art applications of the KKR-GF method allowing them to compare their experiments directly with detailed theoretical predictions and plan further experiments. Existing collaborations have been strengthened and new ones have been established. A large breadth of applications was covered by the experimental speakers and it was established that the KKR-GF is able to deal with a variety of challenging problems to support experimentalists in analyzing their results.

Concerning electronic spectroscopies experimentalists gave clear indication for KKR proponents to work towards descriptions of dynamics. New approaches within KKR to tackle this were discussed. This trend was particularly seen in electronic spectroscopies for time resolved PES and resonant PES. New emerging hybrid systems presented in experimental talks pose new challenges to the DFT-KKR-GF community. In particular, organo-metallic systems that are intensively studied because of their magnetic properties need to be tackled by cutting edge full potential KKR-GF computations.

In the field of magnetism and magnetic fluctuations the KKR-GF already has an extensive track record. However, with the discovery of Skyrmions a new door with many exciting new applications has been opened. Talks by experimentalists made clear that the KKR-GF, in particular in its relativistic version, should be able to treat anisotropic exchange as the foundation for Skyrmion formation. What needs to be done, is the materials- geometry-, and parameter search to tailor robust Skyrmions usable in spintronics. What will also be important is the ability to describe the Gilbert-damping parameter in a truly material specific way. The newly discovered class of topological insulators covered in experimental talks was also discussed in theoretical talks. It turns out that the KKR-GF method is able to go beyond existing model or first-principles supercell calculations, being able to describe semi-infinite multi-component alloy systems and providing theoretical description of electronic spectroscopies. It therefore has the potential to become a powerful tool in finding new TOPOs and guiding experiment.

A treatment of strong electronic correlations within DFT is still a major challenge for any ab-initio electronic structure method. For the KKR several means to include approximations such as the SIC, LSDA+*U* or the DMFT have already been implemented. The talks by the theoreticians gave the experimentalists an insight into the current limits of state-of-the-art first-principles computation and computational based material design for rare earth systems and complex oxides. Concerning electronic transport the KKR-GF method has established its foothold in the community by being able to treat spin-transport and the newly discovered spin Hall effect and thermoelectric effects also discussed in several experimental talks.

Material design for nanoscale systems on a first-principles level is the new upcoming challenge. New methods on how to exploit massively parallel architectures with huge cloud based memory storage will need to be developed. As shown in the workshop the KKR-GF can be adapted for this new paradigm. However the message was conveyed that new programming algorithms have to be invented to take full advantage of these new architectures. Combining all the aforementioned developments for new material

classes (like TOPOs) will enable a versatile and powerful platform to be set up in the future that can be used by a broader user community including electronic structure theoreticians and experimentalists.

The meeting also was part of a series of “Widening Participation” events, driven by EPSRC/CCP9, which aim at building new collaborations between the CCP9 (UK electronic structure) community and new communities, in this case experimental scientists. As part of this “Widening Participation” activity, B. Montanari from STFC joined the discussions as an “external expert”. One of her roles in STFC is to liaise between the scientific computing department of STFC and the STFC facilities (such as ISIS, DIAMOND, etc.) and co-ordinate cross-departmental collaborations. The discussion on widening participation focused on the mechanisms for fostering more collaborative work rather than on specific topics. Several participants would welcome the creation of a network around one of the main application areas that can be studied by the KKR method (e.g., magnetic storage or permanent magnets). The idea of applying for EPSRC funding for the networks was mentioned. Barbara Montanari said that she is exploring the possibility of creating STFC-funded science networks as vehicles for fostering collaborations that also make use of STFC facilities (including the Scientific Computing Department). This was generally seen as a good idea by the participants of the workshop, as it would spread out the effort of writing new proposals and would strengthen the case for proposals when, instead of individuals, whole consortia would bid for new funding.

Annex 4a) Programme of the meeting

Saturday 13 July

13.00 Registration - Physics Concourse, Physics Department (48 on campus map)

13.45 Conference starts - **Physics Lecture Theatre (PLT)** Welcome (Julie Staunton, University of Warwick)

Session 1

14.00 Nicholas Plumb(Swiss Light Source) ***The one-two punch of angle-resolved photoemission and resonant inelasticx-ray scattering: Examples from complex oxides***

14.30 Matti Lindroos (Tampere University of Technology) ***Computational ARPES, beyond spectral functions***

14.55 Friedel Reinert (University of Wuerzburg) ***Kondo and Correlation in Angle Resolved Photoemission Spectroscopy***

15.25 Jurgen Braun (LMU Munich) ***Spectroscopical properties of topological insulators: dichroism, final-state effects and Rashba physics***

15.50 -16.10 Discussion

Coffee (**Physics Concourse**)

Session 2

16.30 Heiko Wende (Universität Duisburg-Essen) ***Magnetic coupling in molecular spin hybrid systems: experiment and theory***

17.00 Samir Lounis (Forschungszentrum Juelich) ***Theory of dynamical magnetic excitations in itinerant nanomagnets***

17.25 Gleb Parakhonskiy (ESRF) ***Search for structure of 3d-metals melts under high pressure with XANES***

17.55 John Rehr (University of Washington) ***Extensions of the Real-space Green's Function Approach for Calculations of* X-ray Absorption and Inelastic Scattering**

18.20 -18.40 Discussion

(Poster boards available)

19.30 Dinner (**Rootes Restaurant**, building 54)

Sunday 14 July

8.45 start

Session 3

8.50 Elizabeth Blackburn (University of Birmingham) ***Interpreting signatures of CDW order in the normal state of underdoped cuprates***

9.20 Martin Gradhand (University of Bristol) ***Kerr rotation and Hall effects in unconventional superconductors***

9.45 Stephen Dugdale (University of Bristol) ***Allying theory to positron annihilation experiments***

10.15 Durga Paudyal (Ames Lab.) ***Rare earth based materials: play ground for theory, computation and experiment***

10.40-11.00 Discussion

Coffee (**Physics Concourse**)

Session 4

11.20 Geetha Balakrishnan (University of Warwick) ***Synthesis and study of Topological Insulators: bulk crystalline and nanomaterials***

11.50 Arthur Ernst (MPI Halle) ***First-principles design of complex oxides***

12.15 Jon Duffy (University of Warwick) ***What can we learn from magnetic Compton scattering?***

12.45-13.00 Discussion

13.00 Lunch (**Rootes Restaurant**, building 54)

13.30-15.00 Posters (**Physics Concourse)**

Session 5

15.00 Jan Honolka (ASCR Prague) ***X-ray absorption spectroscopy of magnetic atoms coupled to topological insulators***

15.30 Peter Krueger (Chiba University) ***Polarization and spin dependent resonant photoemission: what can we learn?***

15.55-16.10 Discussion

Coffee (**Physics Concourse**)

16.30 Saskia Fischer (Humboldt University Berlin) ***Combined structural, electronic and transport investigations of thickness-dependent properties from undoped topological insulator Bi2Se3 microflakes***

17.00 Hubert Ebert (LMU Munich) ***Ab-initio calculation of the Gilbert damping parameter for transition metal alloys by means of a linear response theory***

17.25 Hisazumi Akai (University of Tokyo) ***A new formalism for Keldysh Green's functions in the KKR method***

17.50 Jan Zemen (University of Nottingham) ***Tunneling Anisotropic Magnetoresistance (TAMR) in tunnel junctions with ferromagnetic and antiferromagnetic electrodes***

18.15-18.30 Discussion

19.30 Conference Dinner (**Chancellors Suite, Rootes Building,** 54**)**

Monday 15 July

8.45 start

Session 6

8.50 Khalil Zakeri (MPI Halle) ***Magnetic excitations in ultrathin ferromagnetic films: The***

role of spin-orbit coupling

9.20 Laszlo Szunyogh (Budapest University of Technology and Economics) ***Using the Relativistic Disordered Local Moment scheme for itinerant magnetism at finite temperatures***

9.45 Wulf Wulfhekel (KIT) ***Dynamic magnetic excitations in atoms and clusters - from femto seconds to minutes***

10.15 Ilja Turek (ASCR Brno) ***Tunnelling anisotropic magnetoresistance in epitaxial junctions from ab initio and semi-empirical theory***

10.40-11.00 Discussion

Coffee (**Physics Concourse**)

11.20 Phivos Mavropoulos (Forschungszentrum Juelich) ***Anisotropy of spin relaxation in metals and metallic films***

11.45 Chris Marrows (University of Leeds) ***Spin-polarisation and skyrmions in Co-doped FeSi epilayers***

12.15 -12.30 Discussion

12.30 Lunch (**Physics Concourse**)

Session 7

13.30 Rudi Zeller (Forschungszentrum Juelich) ***KKR Green-function techniques for electronic structure calculations at the nanoscale***

13.55 Christian Heiliger (University Giessen) ***Spin-dependent transport in tunnel junctions with magnetic alloys: Importance of vertex corrections***

14.20 Markus Daene (LLNL) ***Self-Interaction Free and Analytic Treatment of the Coulomb Energy in Kohn-Sham Density Functional Theory***

14.45-15.30 Discussion and closing remarks

15.30-16.00 Coffee (**Physics Concourse**)

16.00-17.00 ***Widening participation*** closed session

Annex 4b) Full list of speakers and participants

Full Name	Affiliation
Alberto Marmodoro	Max-Planck-Institut für Mikrostrukturphysik, Germany
Alexander Edström	Uppsala University, Sweden
Andras Deak	Budapest University of Technology and Economics, Hungary
Arthur Ernst *(Speaker)*	Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany
Barbara Montanari	STFC Rutherford Appleton Laboratory, UK
Biswanath Dutta	Max-Planck-Institut für Eisenforschung GmbH, Germany
Chris Marrows *(Speaker)*	University of Leeds, UK
Christian Franz	University of Giessen, Germany, UK
Christian Heiliger *(Speaker)*	University of Giessen, Germany, UK
Diemo Koedderitzsch	Ludwig-Maximilians-Universität München, Germany
Durga Paudyal *(Speaker)*	The Ames Lab, Iowa State University, USA
Ehsan Barati	Institute of Physical Chemistry of the Polish Academy of Sciences, Poland
Elizabeth Blackburn *(Speaker)*	University of Birmingham, UK
Esha Vinesh Shah	S. V. National Institute of Technology, India.
Fabiana Da Pieve	University of Brussels, Belgium
Fan Pan	Royal Institute of Technology(KTH), Sweden
Francisco Munoz	Max Planck Institute of Microstructure Physics, Halle, Germany
Friedrich Reinert *(Speaker)*	Universität Würzburg, Germany
Gavin Bell	University of Warwick, UK
Geetha Balakrishnan *(Speaker)*	University of Warwick, UK
Gerald Derondeau	Ludwig-Maximilians-Universität München, Germany
Gintare Statkute	None, Lithuania
Gleb Parakhonskiy *(Speaker)*	ESRF, Grenoble, France
Heike Herper	Uppsala University, Sweden
Heiko Wende *(Speaker)*	Universität Duisburg-Essen, Germany
Hisazumi Akai *(Speaker)*	ISSP, The University of Tokyo, Japan
Hubert Ebert *(Speaker)*	Ludwig-Maximilians-Universität München, Germany
Ilja Turek *(Speaker)*	Institute of Physics of Materials, Czech Republic
James Annett	University of Bristol,UK
Jamie Wynn	University of Warwick, UK
Jan Honolka *(Speaker)*	Academy of Sciences of the Czech Republic (ASCR)
Jan Minar	Ludwig-Maximilians-Universität München
Jan Zemen *(Speaker)*	University of Nottingham,UK
John Rehr *(Speaker)*	University of Washington,USA
Jonathan Duffy *(Speaker)*	University of Warwick,UK
Josef Kudrnovsky	Institute of Physics AS CR, Czech Republic
Juergen Braun *(Speaker)*	Ludwig-Maximilians- University, Germany
Julie Staunton	University of Warwick,UK
Khalil Zakeri *(Speaker)*	Max-Planck Institute of Microstructure Physics,Halle, Germany
Konstantinos Koumpouras	Uppsala University, Sweden

Laszlo Szunyogh *(Speaker)*	Budapest University of Technology and Economics,Hungary
Leon Petit	STFC Daresbury Laboratory, UK
Levente Rózsa	Budapest University of Technology and Economics,Hungary
Lukas Wollmann	Max Planck Institute for Chemical Physics of Solids, Germany
Manuel dos Santos Dias	Peter Grünberg Institut (PGI) & Institute for Advanced Simulation (IAS), KFA Juelich, Germany
Markus Daene *(Speaker)*	Lawrence Livermore National Laboratory, USA
Martin Gradhand *(Speaker)*	University of Bristol,UK
Martin Lueders	STFC Daresbury Laboratory, UK
Matti Lindroos *(Speaker)*	Tampere University of Technology, Finland
Mohammed Bouhassoune	PGI1 Forschungszentrum Jülich, Germany
Mohammed Saghir	University of Warwick, UK
Munehisa Matsumoto	ESICMM, NIMS, Tsukuba, Japan
Nicholas Plumb *(Speaker)*	Paul Scherrer Institut, Switzerland
Ondrej Sipr	Institute of Physics ASCR, , Czech Republic
Ouserigha Ebiyibo Collins	University of Warwick,UK
Peter H. Dederichs	Peter Grünberg Institut (PGI) & Institute for Advanced Simulation (IAS), KFA Juelich, Germany
Peter Krüger *(Speaker)*	Chiba University, Japan
Phivos Mavropoulos *(Speaker)*	IAS-1, Forschungszentrum Jülich, Germany
Poulumi Dey	Max-Planck-Institut für Eisenforschung GmbH, Germany
Roman Kovacik	IAS-1, Forschungszentrum Jülich, Germany
Rudolf Sykora	Technical University of Ostrava, Czech Republic
Rudolf Zeller *(Speaker)*	Peter Grünberg Institut (PGI) & Institute for Advanced Simulation (IAS), KFA Juelich
Samir Lounis *(Speaker)*	Peter Grünberg Institut (PGI) & Institute for Advanced Simulation (IAS), KFA Juelich
Saskia Fischer *(Speaker)*	Humboldt University of Berlin, Germany
Shengyen Li	Texas A&M University, USA
Stanislav Chadov	Johannes Gutenberg University of Mainz, Germany
Stephen Dugdale *(Speaker)*	University of Bristol, UK
Sunil Wilfred D'Souza	UGC-DAE Consortium for scientific research, India
Thien Chi Duong	Texas A&M University, Texas, USA
Tuan Khoa Anh Hoang	The University of Glasgow,UK
Vladislav Borisov	Max Planck Institute of Microstructure Physics, Halle, Germany
Wulf Wulfhekel *(Speaker)*	Karlsruhe Institute of Technology, Germany