Vienna Computational Materials Laboratory

ViCoM

VIENNA COMPUTATIONAL MATERIALS LABORATORY

A SPECIAL RESEARCH AREA, FUNDED BY THE AUSTRIAN SCIENCE FUND (FWF)

Sensengasse 8/12, 1090 Vienna, AUSTRIA | t: +43 (0)1 4277-51402 | @: seiichi.chikama@univie.ac.at

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The "Spezialforschungsbereich Vienna Computational Materials Laboratory" ("SFB ViCoM") is a Special Research Area on Computational Materials Science, funded by the Austrian Science Fund (FWF) and managed mainly by researchers of the University of Vienna and the Vienna University of Technology.

The research of the "SFB ViCoM" will mainly focus on an improved description of electronic correlation in solids. The newly developed methods will be applied to cutting-edge materials research using state-of-the-art multi scale methods. The total funding of the "SFB ViCoM" for the first 4 years amounts to 3.9 million euros. For further details, please feel free to contact us.

Key-Note: Facing New Challenges

During the last decades, Computational Science has firmly established its role as an important research tool complementing experimental and theoretical investigations. Materials Science – and especially the novel field of nano-materials – is one of the disciplines where computer simulation methods have played a particularly important role. Progress has been so fast that many current applications could not have been realized five years ago and were hardly dreamed of twenty years ago. Although this development has been facilitated by a rapidly increasing computer performance, the impact of novel theoretical methods in quantum mechanics and statistical mechanics, of improved computational algorithms and of their implementation in highly efficient computer codes has been even more important. With the widening application of computational methods to problems of both fundamental science and modern technology, Computational Materials Science now faces new challenges:

I) The prediction of groundstate total energies and of activation energies of chemical reactions and phase transformations must achieve “chemical accuracy” (i.e. a maximum error of about 1 kcal/mol) for real materials. This requires a substantially improved treatment of many-electron correlations. Here the recent development in the molecular quantum-chemistry has opened new routes, but to achieve the same goal for solids is much more difficult.

II) To maintain the contact with modern experimental Materials Science, the functionality of the existing computer-simulation codes must be extended – detailed predictions of materials properties that can be measured by modern electronic, optical or magnetic spectroscopies in weak and strong fields, as well as the simulation of electronic transport properties must become possible.

III) Even with high-performance computers, the time and lengths scales accessible in the computer-laboratory are many orders of magnitude below those of real-world problems. To bridge these gaps requires the development of multi-scale simulation methods.

Scientists at the University of Vienna and the Vienna University of Technology have made important contributions to the recent progress in Computational Materials Science.

They now combine their forces in the Special Research Area "Vienna Computational Materials Laboratory" confronting the three challenges listed above. We expect that this effort will lead to major advances and breakthroughs in the modeling field.

Dissemination will be through major conferences and through implementation of the developed methods in world-wide used program packages, such as VASP and Wien2k, allowing other researchers and industry to adopt the developed methods in their own research.

Specifically, we will develop and apply a variety of novel methods:

*Ground state of solids: To obtain highly accurate total energies for non-correlated condensed matter (single reference character) we will use coupled-cluster (CC) methods (P02: Towards Exact Correlation in Extended Systems, G. Kresse).

*Ground state and excited states in solids: To describe correlated materials, we aim to merge Dynamical Mean Field Theory (DMFT) and extensions for spatial correlations with advanced DFT methods (P03: Dynamical Mean Field Theory and Beyond, K. Held, P04: Quantum Impurity Solvers, F. Verstraete) and we will develop multi-configuration Hartree-Fock methods for solids (P02: Towards Exact Correlation in Extended Systems, P04: Quantum Impurity Solvers).

*Excited states in molecules and for defects: Development of multi-reference Hartree-Fock (P06: Dynamical Correlated Systems, N. Mauser) and continuation of the development of multi-reference configuration-interaction methods (P05: Embedded Cluster Approach and Non-Adiabatic Processes in Physics and Chemistry, J. Burgdörfer).

*Excited states in solids: For an accurate description of excited states in solids we aim to develop TDDFT methods and many-body perturbation theory (GW + Bethe-Salpeter) (P02: Towards Exact Correlation in Extended Systems, P07: Electronic Structure of Solids, P. Blaha) and embedded multi-reference configuration-interaction methods (P05: Embedded Cluster Approach and Non-Adiabatic Processes in Physics and Chemistry).

*Mathematical foundations: We will develop numerical measures for correlations aiming at a better mathematical understanding of how to distinguish strong correlation from “conventional” weak correlation (P06: Dynamical Correlated Systems).

*Simulation of the magnetic interactions in technologically important materials ranging from an atomic-scale description (P09: Complex Magnetic Structures, P. Mohn) to a suitably parameterized micro-magnetic simulation (P12: Multi-Scale Simulations of Magnetic Nanostructures, D. Suess).

*Simulation of ordering and phase transitions in complex inorganic materials using clusterexpansion and Monte Carlo methods based on parameterized force fields or process parameters derived from ab initio calculations (P10: Multi-Scale Simulations of Multi-Component Phases, R. Podloucky).

*Investigation of self-assembly processes of soft matter and development of improved statistical mechanical sampling techniques such as transition path sampling and genetic algorithms (P11: Nucleation and Self-Assembly in Soft Matter Systems: From the Molecular to the Mesoscopic Scale, Ch. Dellago).

P01: Coordination Project

Project Part Description / Summary

The coordination project will provide the administrative and organizational infrastructure for the SFB. Vital for the external visibility of the SFB, as well as for the internal coherence, is a well organized seminar and colloquium program, with ample room for informal discussion. To strengthen internal collaborations, funds for running a series of small SFB workshops close to Vienna are absolutely necessary. To strengthen the international collaborations and visibility, funds for inviting outstanding international scientists will be crucial.

The main tasks of the coordination project are:

• Management of the administrative tasks within the SFB and reduction of the required management activities of all involved scientists as far as possible. This also involves the coordination of acquiring and installing local computing resources.

• Presentation of the generated knowledge resources (publications, main achievements, developed codes) to a wide public and disseminating the scientific achievements. This includes the maintenance of a well organized WEB page, with up to date information on publications, information on the members of the SFB, and presentations of scientific highlights accessible to a broad audience (experts as well as non experts). In particular, the WEB page should highlight the expertise available in Vienna and developed within the SFB, to forge new academic as well as industrial collaborations.

• Public relation related activities, contact to media, Universities and funding agencies.

• Organization of seminars bi-weekly with ample room for informal discussion in a communicative atmosphere. Particular attention will be placed on regular (twice a month) brief meetings between the principle investigators to discuss new strategies, failures and successes, and to synchronize the individual projects.

• Organization of smaller SFB workshops twice a year with all members of the SFB and a few invited external guests. These small workshops should take place close to Vienna at a site that is sufficiently remote to force close scientific and as well as private interaction between the participants. Emphasize will be placed on ample discussion time (similar to Gordon conferences). From past expertise in National Research Programs, we expect these workshops to become a key factor in forging a strongly interacting research community.

• Organization of one major research workshop and one winter school to consolidate the role of Vienna as a leading center for computational physics and chemistry.

The coordination project will also provide and develop a corporate identity for the computational science groups involved in the SFB, becoming possibly a nucleus for all computational groups in Vienna, maybe even in Austria.

Principal Investigator / Project Part Leader
Univ. Prof. Dipl.-Ing. Dr.
Georg Kresse

Research Partner / National Partner
Univ. Prof. Dipl.-Phys. Dr.
Karsten Held

P02: Towards Exact Correlation in Extended Systems

Project Part Description / Summary

We aim to develop methods for the accurate description of correlation energies in extended systems. The developed methods will be based on a plane-wave expansion of the one-electron wave functions (orbitals), Green's function techniques, in particular the random phase approximation to the correlation energy [Nozières 58], and diagrammatic techniques such as the coupled cluster method [Cizek 1969]. The main goal is to achieve a total energy accuracy that clearly surpasses presently available density functionals, ideally approaching chemical precision (1 kcal/mol). The developed methods should explicitly cover all bonding interactions, i.e., covalent bonding, metallic bonding, dipolar interactions, van der Waals bonding, as well as "strongly correlated systems" (e.g. 3d-metal oxides). They will promote ab-initio techniques for extended systems into a regime that was previously only accessible for small molecules using high level quantum chemistry methods: a way towards truly predictive ab-initio modeling of materials.

Most of the developed methods will explicitly include non-local Hartree-Fock exchange complemented by a suitable correlation functional. The simplest and most straightforward method to construct such functionals is the random phase approximation (RPA) [Nozières 58]. Beyond the RPA, we aim to include electrostatic interactions between particles and holes, possibly particle-particle ladder, and hole-hole ladder diagrams. The developed methods will formally rest on the coupled cluster (CC) method, although specific diagrams of the CC approach (e.g. RPA diagrams) will be evaluated more efficiently using compact integrals on the imaginary frequency axis [Barth 72, Rojas 95, Niquet 03].

During the first four years we specifically plan the following tasks:

- Wave-function based single-reference methods: Coupled cluster code for solids. Fast and numerically stable solver for CCSD equations for solids.

- Efficient methods for the partial summation of selected diagrams, for instance RPA, using imaginary frequency or imaginary time techniques.

- Optimization of single reference state using optimized effective potential (OEP) methods based on the RPA correlation energies.

Since the developed methods are closely linked to methods for quasi-particle and optical excitation energies, such as GW [Hedin 1955] and Bethe-Salpeter [Bethe 1951], the developments will also allow for an improved description of fundamental band gaps and excitation energies. Long term goals are the use of localized Wannier orbitals for the evaluation of correlation energies, exploring links between dynamical mean field theory (exact correlation for Anderson impurity model) and diagrammatic techniques (P03), and the development of multi-reference Hartree-Fock methods for extended systems using matrix product states and/or density matrix renormalization group theory (P04).

Principal Investigator / Project Part Leader
Univ. Prof. Dipl.-Ing. Dr.
Georg Kresse

Principal Investigator / Project Part Leader
Univ. Prof. Dipl.-Ing. Dr.
Georg Kresse

Scientific CV of Georg Kresse

Personal Data

Date of birth: 21.07.1967

Place of birth: Vienna, Austria

Nationality: Austria

University Education

1985-1990: Dipl.-Ing. (Technische Physik), Vienna University of Technology (TUW)

1990-1993 Dr. techn., TUW

Career History

1993-1996 Assistant, Institut für Theoretische Physik, TUW

1996-1997 Postdoc, Keele, University of Staffordshire, UK

1997-1998 Assistant, Institut für Theoretische Physik, TUW

1998-1999 Postdoc, Inst. für Techn. Elektrochemie, TUW

1999-2001 Assistant Professor, Inst. f. Materialphysik, Univ. of Vienna

2001-2007 Associate (Ao.) Professor, Inst. f. Materialph., UV

2007- Univ.-Professor, Computational Quantum Physics, UV

Publications

About 200 refereed publications, H-factor 53

55 invited and plenary lectures at international conferences

Awards

1997 Erich Schmid Award, Austrian Academy of Science

2001 Ludwig-Boltzmann Award, Austrian Physical Society

2003 Start Price of the FWF

2003 Hellmann Price der Internationalen Arbeitsgemeinschaft für Chemie

Research Interests

Heading the development of VASP (Vienna ab initio package).

Ab initio techniques including density functional theory, GW, many-body perturbation theory (MP2), and wave function based correlation methods.

Surface science: growth and oxide formation on metal surfaces.

Nanostructures: ultrathin oxide films, nanotubes, nanodots.

Semiconductor physics: charge trapping, polarons, electronic excitations, defect energies.

Key Publications (Recent 5 Years)

M. Krause, M. Hulman, H. Kuzmany, O. Dubay, G. Kresse, et al., "Fullerene quantum gyroscope", Phys. Rev. Lett. 93, 137403 (2004).

L. Köhler, G. Kresse, M. Schmid, E. Lundgren, J. Gustafson, A. Mikkelsen, M. Borg, J. Yuhara, J. N. Andersen, M. Marsman, and P. Varga, "High-Coverage Oxygen Structures on Rh (111): Adsorbate Repulsion and Site

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G. Kresse, M. Schmid, E. Napetschnig, M. Shishkin, L. Köhler, and P. Varga, "Structure of the Ultrathin Auminum Oxide Film on NiAl(110)", Science 308, 1440 (2005).

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M. Schmid, A. Reicho, A. Stierle, I. Costina, J. Klikovits, P. Kostelnik, O. Dubay, G. Kresse, J. Gustafson, E. Lundgren, J.N. Andersen, H. Dosch, P. Varga, "Structure of Ag(111)-p(4 x4)-O: no silver oxide", Phys. Rev. Lett. 96, 146102 (2006).

M. Shishkin and G. Kresse, "Implementation and performance of frequency-dependent GW method within PAW framework", Phys. Rev. B 74, 035101 (2006).

J. Paier, M. Marsman, K. Hummer, G. Kresse, I.C. Gerber, and J.G. Àngyàn, "Screened hybrid density functionals applied to solids", J. Chem. Phys. 124, 154709 (2006).

K. Hummer, A. Grüneis, and G. Kresse, "Structural and electronic properties of lead chalcogenides from first-principles", Phys. Rev. B 75, 195211 (2007).

F. Fuchs, J. Furthmüller, F. Bechstedt, M. Shishkin, and G. Kresse, "Quasiparticle band structure based on a generalized Kohn-Sham scheme", Phys. Rev. B 76, 115109-1--8 (2007).

J. Paier, M. Marsman, and G. Kresse, "Why does the B3LYP HF/DFT hybrid functional fail for metals?", J. Chem. Phys. 127, 024103 (2007).

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J. Harl, G. Kresse, "Cohesive energy curves for noble gas solids calculated by adiabatic connection fluctuation-dissipation theory", Phys. Rev. B 77, 045136 (2008).

F. Oba, A. Togo, I. Tanaka, J. Paier, and G. Kresse, "Defect energetics in ZnO: A hybrid Hartree-Fock density functional study", Phys. Rev. B 77, 245202 (2008).

A.E. Mattsson, R. Armiento R, J. Paier, G. Kresse, J.M. Wills, and T.R. Mattsson, "The AM05 density functional applied to solids", J. Chem. Phys 128, 084714 (2008).

J. Paier, M. Marsman, G. Kresse, "Dielectric properties and excitons for extended systems from hybrid functional", Phys. Rev. B 78, 121201(R) (2008).

A. Stroppa, and G. Kresse, "The shortcomings of semi-local and hybrid functionals: what we can learn from surface science studies", New J. Phys. 10, 063020 (2008).

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Rojas H N, Godby R W, and Needs R J, 1995, Phys. Rev. Lett. 74, 1827.

Scuseria G E, Henderson T M, and Sorensen D C, 2008, J. Chem. Phys.129, 231101.

Shishkin M, Marsman M, and Kresse G, 2007, Phys. Rev. Lett. 99, 246403.

Stroppa A and Kresse G, 2008, New Journal of Physics 10, 063020.

P03: Dynamical Mean Field Theory and Beyond

Project Part Description / Summary

The accurate calculation of material properties is particularly challenging in the presence of strong electronic correlations as found in transition metal oxides and f-electron systems. In this respect dynamical mean field theory (DMFT) and its merger with density functional theory in the local density approximation (LDA) [Anisimov 97, Lichtenstein 98, Held 07] turned out to be extraordinarily successful. The reason for this success is that DMFT contains a major part of electronic correlations, i.e., the local (quantum) correlations in time. Spatial correlations between different sites (ions), on the other hand, are responsible for many correlation phenomena at low temperature and are neglected in DMFT. In this respect DMFT is still a mean field theory. A major aim of this project is hence to go beyond this mean field level by including short-range and long-range spatial correlations through cluster [Maier 05] and diagrammatic extensions [Toschi 07] of DMFT. To this end the new impurity solvers developed in (P4) will be especially helpful. Through correlation functions, the entropy and the correlation energy, we also plan to determine the degree of correlations included in DMFT and its extension, which needs to be compared to the other beyond-mean-field approaches of this application (also see P6). Another important aim of the project is to integrate DMFT closely into the WIEN2K and VASP program packages (P2 and P7), allowing both for LDA+DMFT and GW+DMFT calculations. To this end both a Wannier function projection and a direct inclusion of Coulomb interaction and correlations within the muffin-tin spheres of the respective APW and PAW wave functions are planned

During the first four years we specifically plan the following tasks:

• integrate DMFT into WIEN2K and VASP through Wannier function projection

• combining DMFT for strong d-d (or f-f) interactions with a screened Hartree-Fock for p-d and p-p interactions

• determine the degree of correlation included in DMFT and its extension by means of simple model Hamiltonians

• estimate the degree of correlations in transition-metal oxides and f-electron materials on the basis of LDA+DMFT, adding LDA and DMFT correlation energy

• application of the developed methods to topical materials

• first feasibility studies for merging LDA and cluster/diagrammatic extensions of DMFT

Long term aims of the project are realistic materials calculations including correlations beyond DMFT and, with a diagrammatic approach such as GW as a starting point, a more thorough calculation of correlations in various material classes.

Principal Investigator / Project Part Leader
Univ. Prof. Dipl.-Phys. Dr.
Karsten Held

Research Partner / National Partner
Univ. Prof. Dr.
Enrico Arrigoni

Principal Investigator / Project Part Leader
Univ. Prof. Dipl.-Phys. Dr.
Karsten Held

Scientific CV of Karsten Held

Personal Data

Date of birth: 20.07.1971

Place of birth: Clausthal-Zellerfeld, Germany

Nationality: Germany

University Education

1990 – 1995 Physics studies at the RWTH Aachen, Germany

1995 Diploma in Physics, RWTH Aachen with distinction

1999 Ph.D. in Physics, Augsburg University, with distinction

Career History

1995 – 1996 Research assistant, RWTH Aachen and (compulsory) civilian service, IME, FZ Jülich

1996 – 2000 Research assistant, Augsburg University

1998 DAAD research fellow, UC Davis

2000-2002 Alexander von Humboldt fellowship, Princeton University

2002-2008 Head of Emmy-Noether group, Max Planck Institute for Solid State Research, Stuttgart

2004 Habilitation in theoretical physics, Stuttgart

2008 - Full professor, Institute for Solid State Physics, TU Vienna

Publications

More than 55 publications with approx 1250 citations, H-factor=20, more than 60 invited talks

Awards

1996 Springorum Münze and Friedrich Wilhelm Prize of the RWTH Aachen

1998 DAAD fellowship

2000 Feodor Lynen grant of the Alexander von Humbold-Stiftung

2002 Emmy Noether grant of the German Science Foundation (DFG)

Research Interests

Strongly-correlated electron systems, computational materials science, physics of correlated electron systems, nanostructures, magnetism, superconductivity, electron dynamics, decoherence.

Key Publications (Recent 5 Years)

P. Hansmann, X. Yang, A. Toschi, G. Khaliullin, O. K. Andersen, and K. Held, “Turning a nickelate Fermi surface into a cuprate-like one through heterostructuring”, Phys. Rev. Lett.103, 016401 (2009).

A. Toschi, M. Capone, C. Castellani and K. Held, ”Kinks in the electronic specific heat”, Phys. Rev. Lett. 102, 076402 (2009).

A. Hübel, K. Held, J. Weis and K. v. Klitzing, “Correlated electron tunneling through two separate quantum dot systems with strong capacitive interdot coupling”, Phys. Rev. Lett. 101, 186804 (2008).

R. Arita, K. Kuroki, K. Held, A. V. Lukoyanov, S. Skornyakov and V.I. Anisimov, "Origin of

large thermopower in LiRh2O4", Phys. Rev B. 78, 115121 (2008).

A. Toschi, A. A. Katanin and K. Held, "Dynamical vertex approximation - a step beyond dynamical mean field theory", Phys. Rev. B 75, 045118 (2007).

R. Arita, K. Held, A.V. Lukoyanov and V.I. Anisimov, "Doped Mott insulator as the origin of heavy Fermion behavior in LiV2O4", Phys. Rev. Lett. 98, 166402 (2007).

K. Byczuk, M. Kollar, K. Held, Y.-F. Yang, I. A. Nekrasov, Th. Pruschke and D. Vollhardt, "Kinks in the dispersion of strongly correlated electrons", Nature Physics 3, 168 (2007).

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A. Yamasaki, M. Feldbacher, Y.-F. Yang, O. K. Andersen and K. Held, Pressure-induced metal-insulator transition in LaMnO3 is not of Mott-Hubbard type, Phys. Rev. Lett. 96, 166401 (2006).

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K. Held, I. A. Nekrasov, G. Keller, V. Eyert, N. Blümer, A. K. McMahan, R. T. Scalettar, Th. Pruschke, V. I. Anisimov and D. Vollhardt, "Realistic investigations of correlated electron systems with LDA+DMFT", Physica Status Solidi B 243, 2599 (2006) (review article).

R. Arita and K. Held, "Orbital-selective Mott-Hubbard transition in the two-band Hubbard model", Phys. Rev. B 72, 201102 (R) (2005).

A. Sekiyama, H. Fujiwara, S. Imada, S. Suga, H. Eisaki, S. I. Uchida, K. Takegahara, H. Harima, Y. Saitoh, I. A. Nekrasov, G. Keller, D. E. Kondakov, A. V. Kozhevnikov, Th. Pruschke, K. Held, D. Vollhardt and V. I. Anishimov, "Mutual Experimental and Theoretical Validation of Bulk Photoemission Spectra of Sr1-xCaxVO3", Phys. Rev. Lett. 93, 156402 (2004).

M. Feldbacher, K. Held and F. F. Assaad, "Projective Quantum Monte Carlo Method for the Anderson Impurity Model and its Application to Dynamical Mean Field Theory", Phys. Rev. Lett. 93, 136405 (2004).

S.-K. Mo, H.-D. Kim, J. W. Allen, G.-H. Gweon, J. D. Denlinger, J.-H. Park, A. Sekiyama, A. Yamasaki, S. Suga, P. Metcalf and K. Held, "Filling of the Mott-Hubbard gap in the high temperature photoemission spectrum of (V0.972Cr0.028)2O3", Phys. Rev. Lett. 93, 76404 (2004).

Research Partner / National Partner
Univ. Prof. Dr.
Enrico Arrigoni

Scientific CV of Enrico Arrigoni

Personal Data

Date of birth: 28.01.1966

Place of birth: Treviso, Italy

Nationality: Italy

University Education

1984 – 1993	Physics studies at the University of Pisa and at the Scuola Normale Superiore. Pisa, Italy
1989	Laurea (Degree) in Physics summa cum laude
1993	Ph.D. in Physics summa cum laude

Career History

1989 – 1992	Scholarship by Europa Metalli LMI
1992 – 1993	Civil Service (at Caritas, Pisa)
1994 – 1995	Post doc at the Max-Planck Institute Stuttgart
1995 – 2001	Postdoc and from 1998 research assistant at the University of Würzburg
2000	Habilitation in Theoretical Physics, University of Würzburg
2001-2003	Heisenberg Fellowship from the DFG: research stays at the University of Würzburg, at Stanford University, at the University of California Los Angeles and at the University of Geneva
2003 -	Univ. Prof., Institute of Theoretical and Computational Physics, Graz University of Technology

Publications

87 refereed publications, appr. 900 citations, h-index=20, 21 invited talks at international conferences

Research Interests

Strongly-correlated condensed-matter systems, High-Temperature superconductors, orbitally degenerate materials, Half-metallic ferromagnets, Low-dimensional conductors and dimensional crossover. Development of numerical methods for strongly-correlated systems.

Key Publications (Recent 5 Years)

H. Allmaier, L. Chioncel , and E. Arrigoni, “Titanium Nitride - a correlated metal at the threshold of a Mott transition”, arXiv:0904.3569, accepted for publication in Phys. Rev. B (2009).

Xiancong Lu , and E. Arrigoni, “Dispersive spectrum and orbital order of spinless p-band fermions in an optical lattice”, Phys. Rev. B (2009).

S. Brehm, E. Arrigoni, M. Aichhorn , and W. Hanke, “Consistent description of magnetic excitations and the phase diagram”, in the strongly - correlated Hubbard model of high-Tc cuprates, arXiv:0811.0552 (2008).

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E. Arrigoni, E. Fradkin , and S. A. Kivelson, “Mechanism of High Temperature Superconductivity in a striped Hubbard Model”, Phys. Rev. B 69, 214519 (2004).

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P04: Quantum Impurity Solvers

Project Part Description / Summary

The problem of simulating quantum impurities has since long played a central role in the field of condensed matter physics and more specific in the context of strongly correlated quantum systems. Besides the fundamental and independent interest and relevance of that problem, the simulation of the spectral functions of quantum impurities is currently receiving a large amount of attention as it forms the core of the so-called dynamical mean field theory [Georges 05] (DMFT) methods for simulating general correlated materials (see P3). The state of the art method for solving such impurity problems is based on quantum Monte Carlo simulations [Rubtsov 05, Werner 06], but numerical renormalization group methods have also proven to form a valuable tool [Bulla 08].

In recent years, insights coming from the field of quantum information theory have redefined the way numerical re-normalization group methods can be applied and considerably extended their range of applicability; those methods are based on the concept of matrix product states (MPS) and bear the promise to solve seminal open problems such as the determination of the phase diagram of the Hubbard model [Verstraete 08]. The central goal of this proposal is to use those new tools, and specifically the novel time-evolution algorithms [Daley 05, Verstraete 04], to develop methods for simulating the spectral properties of quantum impurity problems. One of the main incentives for doing so stems from our experience of the closely related problem of simulating quantum spin systems, in which the MPS-methods outperform Monte Carlo based methods [Verstraete 05, Schollwöck 06].

One of the main advantages of the MPS-approach is its scalability by construction. This is of central importance in the context of the DMFT-related applications, where a large improvement of the applicability and precision is expected when large clusters of impurities can be simulated instead of small ones. Given the similarity of this problem to the problem of simulating quantum lattice Hamiltonians, we will explore how to apply matrix product states and its generalizations to those cluster DMFT problems. The main advantage is that the MPS-based methods are not plagued by the sign problem, which is the main reason why large clusters are out of reach of Monte Carlo methods.

Clearly, this project will be done in close collaboration with Project Held (P3), but the topic of impurity solvers is of much wider interest. The techniques that we are planning to use could be very useful in the context of multi-configuration Hartree-Fock methods (P2) and to P6, where a theoretical framework will be built to get a better understanding of the concept of quantum correlations.

Principal Investigator / Project Part Leader
Univ. Prof. Dr.
Frank Verstraete

Research Partner / National Partner
Ao. Univ. Prof. Dipl.-Phys. Dr.
Hans Gerd Evertz

Principal Investigator / Project Part Leader
Univ. Prof. Dr.
Frank Verstraete

Scientific CV of Frank Verstraete

Personal Data

Date of Birth: 14.11.1972

Place of Birth: Izegem, Belgium

Nationality: Belgian

Scientific Education

Oct 91 – Jun 96	Masters degree in Electrical Engineering at the University of Leuven
Oct 96 – Jun 98	Masters degree in Theoretical Physics at the University of Ghent
Jul 98 – Oct 02	PhD with title "A study of entanglement in quantum information theory" at the University of Leuven

Career History

Oct 02 – Sep 04	Research fellow in the theory group of Prof. J.I. Cirac at the Max Planck Institut für Quantenoptik
Oct 04 – Sep 06	Research Scholar in the Institute for Quantum Information headed by Prof. J. Preskill at Caltech
Since Oct 06	Full Professor, faculty of Physics. University of Vienna

Awards

2005 Academische Stichting Leuven (ASL) prijs exacte wetenschappen

2007 Hermann Kümmel early achievement award in many-body physics

Publications

Number of publications in refereed journals: 71 (H-index: 26)

Invited conference talks: 25

Research Interests

Quantum Information Theory and the Theory of Entanglement

Strongly Correlated Quantum Systems

Simulation of strongly correlated quantum systems

Computational Complexity

Key Publications (Recent 5 Years)

F. Verstraete, D. Porras, J.I. Cirac, "DMRG and periodic boundary conditions: a quantum information perspective", Phys. Rev. Lett. 93, 227205 (2004).

F. Verstraete, J. J. Garcia-Ripoll, J.I. Cirac, "Matrix Product Density Operators: Simulation of finite-T and dissipative systems", Phys. Rev. Lett. 93, 207204 (2004).

V. Murg, F. Verstraete, J. I. Cirac, "Efficient evaluation of partition functions of inhomogeneous many-body spin systems", Phys. Rev. Lett. 95, 057206 (2005).

B. Paredes, F. Verstraete, J. I. Cirac, "Exploiting Quantum Parallelism To Simulate Quantum Random Many-Body

Systems", Phys. Rev. Lett. 95, 140501 (2005).

F. Verstraete, J.I. Cirac, "Mapping local Hamiltonians of fermions to local Hamiltonians of spins", J. Stat. Mech., P09012 (2005).

F. Verstraete, A. Weichselbaum, U. Schollwock, J.I. Cirac and J. von Delft, condmat/0504305v2 (2005).

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V. Murg, F. Verstraete, J. I. Cirac, "Variational study of hard-core bosons in a 2-D optical lattice using Projected Entangled Pair States (PEPS)", Phys. Rev. A 75, 033605 (2007).

F. Verstraete, V. Murg, J.I. Cirac, "Matrix product states, projected entangled pair states, and variational renormalization group methods for quantum spin systems", Adv. in Phys. 57, 143 (2008)

Research Partner / National Partner
Ao. Univ. Prof. Dipl.-Phys. Dr.
Hans Gerd Evertz

Scientific CV of Hans Gerd Evertz

Personal Data

Date of Birth: 19.03.1959

Place of Birth: Heinsberg, Germany

Nationality: German

Scientific Education

Oct 77 – May 83	Diploma in physics and bachelor in computer science, RWTH Aachen
Sep 83 – Aug 84	Visiting scholar, Stanford University
Sep 84 – Sep 87	Ph.D., Theoretical physics ("Lattice analysis of the Higgs mechanism")
Jun 00	Habilitation (Theoretical physics, TU Graz)

Career History

1987 – 1990	Wiss. Mitarbeiter (postdoc), Univ. Hamburg
1990 – 1993	Postdoctoral Research Associate, Supercomputer Computations Research Institute, Florida State University
1993 – 1995	Postdoctoral Fellow, Center for Simulational Physics, Univ. of Georgia
1995 – 1999	Wiss. Mitarbeiter, Univ. Würzburg
1999 – 2000	Universitätsassistent, TU Graz
2000 – present	Ao. Univ.Prof., TU Graz

Scholarships

1980 – 1981	Scholarship from Fritz ter Meer Stiftung
1981 – 1983	Studienstiftung (German National Scholarship Foundation)
1983 – 1984	Research Scholarship for Stanford University
1985 – 1987	Ph.D. Scholarship from Studienstiftung

Publications

Number of publications in refereed journals: 53 (H-index: 16)

Research Interests

Strongly correlated quantum systems (spins, bosons, electrons)

Simulations, new algorithms, exact mappings

Real time evolution

Quantum Monte Carlo techniques

Quantum Field Theory

Selected Project Relevant Publications for Hans Gerd Evertz

P. Pippan, S.R. White, and H.G. Evertz, "Improved Scaling for Periodic Matrix Product State Algorithms", to appear in Phys. Rev. B (Rapid Commun.)

P.Pippan, H.G. Evertz, and M. Hohenadler, "Dynamics of strongly correlated lattice

bosons and polaritons in one dimension" (Cavity photons), arxiv:0904.1350.

A.W. Sandvik and H.G. Evertz, "Loop updates for valence-bond projector quantum Monte Carlo simulations", arxiv:0807.0682, to appear in Phys. Rev. B.

F.F. Assaad and H.G. Evertz, "World line and determinantal Quantum Monte Carlo methods for spins, phonons, and electrons", Springer Lecture Notes in Physics 739, ed. H. Fehske et al. (2008)

B. Edegger, H.G. Evertz, and R.M. Noack, "Creation and destruction of a spin gap in weakly coupled quarter-filled ladders" (DMRG), Phys. Rev. Lett. 96, 146401 (2006)

D.R. Neuber, M. Daghofer, H.G. Evertz, W. von der Linden, and R.M. Noack, "Ferromagnetic polarons in the one-dimensional ferromagnetic Kondo model with quantum mechanical S=3/2 core spins" (DMRG), Phys. Rev. B73, 014401 (2006)

B. Edegger, H.G. Evertz, and R.M. Noack, "Charge order induced by electron-lattice interaction in NaV2O5" (DMRG), Phys. Rev. B72, 085131 (2005)

M. Aichhorn, E.Ya. Sherman, and H.G. Evertz, "Single-particle spectral function of quarter-filled ladder systems", Phys. Rev. B72, 155110 (2005)

M. Daghofer, M. Konneger, H.G. Evertz, and W. von der Linden, „Perfect Tempering", AIP Conf. Proc. 735, 355 (2004)

M. Aichhorn, M. Daghofer, H.G. Evertz, and W. von der Linden, "Low Temperature Lanczos Method for strongly correlated systems", Phys. Rev. B67, 161103R (2003)

H.G. Evertz and W. von der Linden, "Simulations on Infinite Size Lattices", Phys. Rev. Lett. 86, 5164 (2001)

H.G. Evertz, "The Loop Algorithm", Advances in Physics 52, 1-66 (2003)

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Verstraete F. et al., condmat/0504305 (2005).

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Bañuls M.C. et al., to be published in Phys. Rev. Lett. (2009)

P05: Embedded Cluster Approach and Non-Adiabatic Processes in Physics and Chemistry

Project Part Description / Summary

The High-level wavefunction based methods will be employed within the framework of an embedded cluster approach (ECA) to study strongly localized defects and excitations in solids and at surfaces as well as the ensuing dynamical processes on fast timescales. The ECA allows the implementation of state-of-the-art quantum mechanical techniques beyond mean-field descriptions to scenarios where correlation effects in excited states are crucial and where the Born-Oppenheimer approximation, the foundation of most quantum mechanical simulations, breaks down.

The strength of high-level quantum chemistry methodology such as multi-reference configuration interaction (MRCI) and multi-configuration self-consistent field (MCSCF) methods lies in the ability to account for strong correlations of localized electrons. Its application has been typically limited to relatively small molecules in view of the unfavorable, generally exponential scaling with size. This barrier can be overcome on an approximate level by embedding the active cluster into a matrix of a larger finite or extended system. First applications to wide-band insulators indicate that properties of extended systems such as the valence band structure can be accurately represented for computationally realistic sizes of embedded clusters. This opens up new opportunities to simulate the correlated dynamics of localized defects, excitons, trionic excitations, and excited-state relaxation in clusters, surfaces and solids.

As a long-term goal we aim at full dynamical simulations starting with the primary excitation process, following the evolution of the coherently excited many-body electronic state and its relaxation. This requires the implementation of non-adiabatic couplings between energy hypersurfaces within the framework of "on-the fly" surface hopping dynamics and with an open quantum system (OQS) approach, the quantum trajectory Monte Carlo (QTMC) method, to account for environmental degrees of freedom.

During the first four years we will focus on:

• Benchmarking the ECA against state-of the art DFT and post-DFT methods for extended systems applied to localized excitations in wide-band gap insulators.

• Computation of accurate reference data and determination of effective tight-binding parameters for structural defects, local edge disorder and adsorbates.

• Integrating the ECA, non-adiabatic dynamics, and QTMC methods.

• Simulating non-adiabatic processes in charged-particle-alkalihalide scattering and photo- and defect dynamics in DNA.

Principal Investigator / Project Part Leader
o. Univ. Prof. Dipl.-Phys. Dr.
Joachim Burgdörfer

Research Partner / National Partner
Univ. Prof. i. R. Dr.
Hans Lischka

Principal Investigator / Project Part Leader
o. Univ. Prof. Dipl.-Phys. Dr.
Joachim Burgdörfer

Scientific CV of Joachim Burgdörfer

Personal Data

Date of birth: 22.06.1953

Place of birth: Tennenbronn

Nationality: Germany / Austria

University Education

1972 – 1982	Freie Universität Berlin, Department of Physics
1978	Diploma in Physics summa cum laude
1982	Ph.D. in Theoretical Physics summa cum laude

Career History

1982 – 1983	Visiting Scientist (postdoc), Oak Ridge National Laboratory, Oak Ridge, Tennessee
1983 – 1984	Instructor , Freie Universität Berlin
1984 – 1995	Ass. Prof., Assoc . Prof. and Full Professor (since 1988), Department of Physics, University of Tennessee
1986 – 1997	Adjunct Research Staff Member ORNL
1995 – 2000	(1997 - 2000 on leave) Alumni Distinguished Professor of Physics, University of Tennessee
1997 -	O.Univ.Prof., Institute for Theoretical Physics, TUW
2004 -	Director, Institute for Theoretical Physics, TUW

Publications

More than 300 refereed publications, h-index 35

More than 100 invited lectures at international conferences

Awards

1993	Elected Fellow of the American Physical Society
1993	Chancellor's Award for Research and Creative Achievement
2001	Elected Corresponding Member of the Austrian Academy of Sciences
2004	RIKEN Eminent Scientist Award (Japan)
2005	Elected Full Member of the Austrian Academy of Sciences

Research Interests

Photon and charged particle interactions with solids and surfaces, quantum transport, attosecond physics, open-quantum system description, non-linear dynamics

Key Publications (Recent 5 Years)

J. Güttinger, C. Stampfer, F. Libisch, T. Frey, J. Burgdörfer, T. Ihn, and K. Ensslin, "Electron-Hole Crossover in Graphene Quantum Dots"; Phys. Rev. Lett., accepted (2009).

C. Lemell, B. Solleder, K. Tőkési, and J. Burgdörfer, "Simulation of attosecond streaking of electrons emitted from a tungsten surface"; Physical Review A 79, 062901 (2009).

K. Schiessl, K. Tőkési, B. Solleder, C. Lemell, and J. Burgdörfer, "Electron Guiding through

Insulating Nanocapillaries"; Physical Review Letters 102, 63201 (2009).

F. Libisch, C. Stampfer, and J. Burgdörfer, "Graphene quantum dots: Beyond a Dirac billiard"; Physical Review B 79, 115423 (2009).

B. Solleder, L. Wirtz, and J. Burgdörfer: „Vanishing gap in LiF for electronic excitations by slow antiprotons";Phys. Rev. B 79, 125107 (2009).

F. Aigner, N. Simonović, B. Solleder, L. Wirtz, and J. Burgdörfer, "Suppression of Decoherence in Fast-Atom Diffraction at Surfaces"; Phys. Review Letters 101, 253201 (2008).

C. Prigent, C. Deiss, E. Lamour, J.-P. Rozet, D. Vernhet, and J. Burgdörfer, "Effect of pulse duration on the x-ray emission from Ar clusters in intense laser fields"; Physical Review A 78, 053201 (2008).

A.S. El-Said, R. Heller, W. Meissl, R. Ritter, S. Facsko, C. Lemell, B. Solleder, I. Gebeshuber, G. Betz, M. Toulemonde, W. Möller, J. Burgdörfer, F. Aumayr, "Creation of Nanohillocks on CaF2 Surfaces by Single Slow Highly Charged Ions"; Physical Review Letters 100, 2376011 (2008).

B. Solleder, L. Wirtz, J. Burgdörfer, "Excitation energy and pair correlation function of trions near a LiF surface"; Physical Review B 78, 155432 (2008).

F. Libisch, J. Möller, S. Rotter, M. Vavilov, J. Burgdörfer, "Decreasing excitation gap in Andreev Billiards by disorder scattering";European Physics Letters 82, 47006 (2008).

J. Feist, A. Bäcker, R. Ketzmerick, S. Rotter, B. Huckestein, J. Burgdörfer, "Nanowires with surface disorder: Giant localization lengths and quantum-to-classical crossover"; Physical Review Letters 97, 116804 (2006)

F. Aigner, S. Rotter, J. Burgdörfer, "Shot noise in the chaotic-to-regular crossover regime"; Physical Review Letters 94, 21680 (2005).

M. Seliger, C. O. Reinhold, T. Minami, J. Burgdörfer, "Nonunitary quantum trajectory Monte Carlo method for open quantum systems"; Physical Review A 71, 062901 (2005).

A. Apolonski, P. Dombi, G.G. Paulus, M. Kakehata, R. Holzwarth, T. Udem, C. Lemell, J. Burgdörfer, T. Hänsch, F. Krausz, "Observation of light-phase-sensitive photoemission from a metal surface"; Physical Review Letters 92, 073902 (2004).

L. Wirtz, M. Dallos, H. Lischka, and J. Burgdörfer, "Ab-initio Calculations of Charge Exchange in Ion-surface Collisions: An Embedded-cluster Approach" in: Correlation Spectroscopy of Surfaces, Thin Films, and Nanostructures, edited by J. Berakdar and J. Kirschner, Wiley-Weinheim, pp. 130-144, (2004).

Research Partner / National Partner
Univ. Prof. i. R. Dr.
Hans Lischka

Scientific CV of Hans Lischka

Personal Data

Date of birth: 26.07.1943

Place of birth: Vienna, Austria

Nationality: Austria

University Education

1961-1969 Ph.D. study at the University of Vienna

Career History

1968-1969 Teaching Assistant, Institute for Theoretical Chemistry, University of Vienna, Austria

1969-1976 Assistant at the Institute for Theoretical Chemistry and Radiation Chemistry, University of Vienna

1972-1973 Postdoc (Humboldt fellowship) with W. Kutzelnigg, University of Karlsruhe, Germany

1976 Habilitation at the University of Vienna

1976-1980 Assistant Professor, Institute for Theoretical Chemistry and Radiation Chemistry, University of Vienna

1980-2008 Professor at the same institute

1992-1996 Director of the Institute for Theoretical Chemistry and Radiation Chemistry, University of Vienna

1993-1995 Head of the section for Vienna, Lower Austria and Burgenland of the Austrian Chemical Society

2000-2001 Chairman of the Austrian Chemical Physical Society

Publications

About 200 refereed publications, h-index 42

100 invited and plenary lectures at international conferences

Awards

1971 Award Prize from the Theodor-Körner Foundation

1980 Sandoz Prize for Chemistry

2008 Special Issue Chemical Physics 349 (2008) in honor of 65th birthday of Hans Lischka

Research Interests

Development of high-level quantum chemical methods within the COLUMBUS project, nonadiabatic surface-hopping dynamics, Computational Photochemistry and Photobiology, Adsorption studies in Soil Science

Key Publications (Recent 5 Years)

L. Wirtz, J. Burgdörfer M. Dallos, Th. Müller, and H. Lischka, “Potential energy surfaces for charge exchange between singly charged ions and a LiF surface”, Phys. Rev. A, 68, 32902 (2003).

G. F. Bauerfeldt, and H. Lischka, “A Multireference CI Study on Excitation Energies and Potential Energy Surfaces of CH3F”, J. Phys. Chem. A, 108, 3111 (2004).

H. Lischka, M. Dallos, P. G. Szalay, D. R. Yarkony, and R. Shepard, “Analytic evaluation of nonadiabatic coupling terms at the MRCI level. I: Formalism”, J. Chem. Phys., 120, 7322 (2004).

M. Dallos, H. Lischka, R. Shepard, D. R. Yarkony, and P. G. Szalay, “Analytic evaluation of nonadiabatic coupling terms at the MRCI level. II. Minima on the crossing seam: formaldehyde and the photodimerization of ethylene”, J. Chem. Phys., 120, 7330 (2004).

D. Tunega, M. H. Gerzabek, and H. Lischka, “Ab initio molecular dynamics study of a monomolecular water layer on octahedral and tetrahedral kaolinite surfaces”, J. Phys. Chem. B, 108, 5930 (2004).

A. J. A. Aquino, H. Lischka, and Ch. Hättig, “Excited-State Intramolecular Proton Transfer: A Survey of TDDFT and RI-CC2 Excited-State Potential Energy Surfaces”, J. Phys. Chem. A, 109, 3201 (2005).

W. J. D. Beenken, and H. Lischka, “Spectral Broadening and Diffusion by Torsional Motion in Biphenyl”, J. Chem. Phys., 123, 144311 (2005).

R. Mitrić, V. Bonačić-Koutecký, J. Pittner, and H. Lischka, “Ab initio nonadiabatic dynamics study of ultrafast radiationless decay over conical intersections illustrated on the Na3F cluster”, J. Chem. Phys., 125 024303 (2006).

M. Barbatti, G. Granucci, M. Persico, M. Ruckenbauer, M. Vazdar, M. Eckert-Maksić, and H. Lischka, “The on-the-fly surface-hopping program system NEWTON-X: application to ab initio simulation of the nonadiabatic photodynamics of benchmark systems”, Journal of Photochemistry and Photobiology A, 190, 228 (2007).

M. Barbatti, and H. Lischka, “Can the nonadiabatic photodynamics of aminopyrimidine be a model for the ultrafast deactivation of adenine?”, J. Phys. Chem. A, 111, 2852 (2007).

V. Lukeš, A. J. A. Aquino, H. Lischka, and H.-F. Kauffmann, “On the dependence of optical properties of oligo-para-phenylenes on torsional modes and chain length”, J. Phys. Chem. B, 111, 7954 (2007).

Perspectives Article: Mario Barbatti, Matthias Ruckenbauer, Jaroslaw J. Szymczak, Adélia J. A. Aquino, and Hans Lischka, “Nonadiabatic excited-state dynamics of polar □-systems and related model compounds of biological relevance”, PhysChemChemPhys, 10, 482 (2008).

Ch. Schriever, M. Barbatti, K. Stock, A. J. A. Aquino, D. Tunega, St. Lochbrunner, E. Riedle, R. de Vivie-Riedle, and H. Lischka, “The interplay of skeletal deformations and ultrafast excited state intramolecular proton transfer: experimental and theoretical investigation of 10-hydroxybenzo[h]quinoline”, Chem. Phys. 347, 446 (2008).

M. Barbatti, and H. Lischka, “The non-adiabatic deactivation of 9H-adenine: a comprehensive picture based on mixed quantum-classical dynamics”, J. Am. Chem. Soc. 130, 6831 (2008).

J. Pittner, H. Lischka, and M. Barbatti, “Optimization of mixed quantum-classical dynamics: time-derivative coupling terms and selected couplings”, Chem. Phys. 356, 147 (2009).

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Harl J and Kresse G, 2008, Phys. Rev. B 77, 045136.

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Lukeš V, Šolc R, Barbatti M, Elstner M, Lischka H, et al., 2008, JCP 129, 164905.

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P06: Dynamical Correlated Systems

Project Part Description / Summary

This project is devoted to methods for strongly correlated electron dynamics that arose, e.g., in the new field of ultra-fast pump-probe type spectroscopy [Scrinzi 2006, Cavalieri 2008]. We will investigate fundamental questions like measures for correlation and its role in dynamics and we will construct new methods by combining multi-configuration time-dependent Hartree-Fock (MCTDHF, [Zanghellini 2003, Caillat 2005, Nest 2005, Bardos 2009]) with many-body methods employed by us (TDDFT) and other groups (GW, DMFT) within this SFB. Although TDDFT is a general time-dependent method, its successful applications are in the linear-response regime, while – at least in its present realizations – it faces severe limitations in the description of excited dynamics, which may be related to the very foundations of TDDFT [e.g. Maitra 2002]. MCTDHF in principle allows systematic convergence towards the exact solution, but requires large computational resources and is currently limited to moderate particle numbers (<10) because of its unfavorable scaling. Our developments during the first SFB period will be aimed at three applications: (1) ab-initio few-electron dynamics: a) atoms in external fields b) quantum dots (2) small molecules: a) LiF with moving nuclei b) quantum dot molecules (3) field-induced dynamics at solid surfaces.

We group our work into 4 areas:

Concepts: Contribute to a unified concept of correlation. Apply existing measures and develop new measures for correlation that are meaningful in the context of methods used across the SFB; understand foundations of TDDFT and MCTDHF and the link between them (collaboration with P2, P3, and P4).

New methods: Improve the scaling of MCTDHF by systematic approximations; integrate MCTDHF and its derivatives with TDDFT and GW for adiabatic background dynamics (with P2 and P5). Combine MCTDHF and TDDFT with classical dynamics for nuclei.

Applications: Benchmark the approximative methods on simple molecular systems. Apply the new methods to (systems of) charged quantum dots, small molecules and ultra-fast emission by localized fields.

Advanced algorithms: Single-particle discretization by tensor-product expansions of moderately correlated degrees of freedom; self-adaptive hierarchical matrix methods for two-particle interactions; time-integrators; absorbing boundary conditions.

A long term objective of the project is to narrow the gap between highly developed computational tools for the stationary (and linear response) regime and few- and multi-electron dynamics calculations by incorporating techniques from the former into the latter. We see an additional task in advancing numerical and computational techniques for applications across the SFB.

Principal Investigator / Project Part Leader
Ao. Univ. Prof. Dr.
Norbert J. Mauser

Research Partner / National Partner
Prof. Univ. Doz. Mag. Dr.
Armin Scrinzi

Principal Investigator / Project Part Leader
Ao. Univ. Prof. Dr.
Norbert J. Mauser

Scientific CV of Norbert J. Mauser

Personal Data

Homepage: www.wpi.ac.at/director.html

Date, place of birth, nationality: 03.08.1964, Wien, Österreich

University Education

1982-1990	Dipl.-Ing. (Techn. Mathematik & Techn. Physik, TU Wien) and B.S. (Astronomy, Uni Wien)
1990-1994	Dr. techn., TU Wien
1999	Habilitation in Mathematik, Uni Wien

Career History

1988-1991	Research Associate, Inst. f. Theor. Physik and Inst. f Angew. & Numerische Math, TU Wien
1984-1985	Military service
1991-1996	Assistant (wiMi), TU Berlin, Appl. Math group
1993-1994	Researcher, CRS4, Cagliari, Italy, Num. Simulation group
1996-1997	Postdoc, Univ. Nice, France
1998-1999	Postdoc, Courant Inst., New York Univ.
1997-1999	Ass.Prof., Inst. f. Math., Uni Wien (on leave)
1999-	Ao.Univ.Prof., Fak.Math, Uni Wien

Publications

About 80 refereed papers, h-factor 17 (mathematics)

40 invited and plenary lectures at international conferences

Awards

1995	Marie Curie Fellowship of the EU 4th Framework Programme
1996	Schrödinger Stipendium of the FWF
1999	START Prize of the FWF
2000	Prize of the Austrian Math. Society

Research Interests

Mathematical modeling and analysis, numerics and simulation of time dependent partial differential equations in quantum physics, concepts of correlation, TDDTF, MCTHDF

Key Publications (Recent 5 Years)

W. Bao, N.J. Mauser and H.P. Stimming, “Effective one particle quantum dynamics of electrons : the Schrödinger-Poisson-Xalpha model”, Comm. Math. Sci. 1 (4) (2003) 809—831

C. Bardos, F. Golse, A. Gottlieb and N.J. Mauser, “Accuracy of the time-dependent Hartree-Fock approximation for uncorrelated initial states”, J. Stat. Phys. 115 (3/4) (2004) 1037 – 1055

P. Bechouche, N.J. Mauser and S. Selberg, “On the asymptotic analysis of the Dirac-Maxwell system in the nonrelativistic limit”, J. Hyp.Diff. Equ. 2 (1) (2005) 129 – 182

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L. Gosse and N.J. Mauser, "Multiphase semiclassical approximation of an electron in a one-dimensional crystalline lattice III : WKB for Schrödinger-Poisson", J. Comp. Phys. 211(1) (2006) 326-346

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N. Besse, N.J. Mauser and E. Sonnendrucker, "Numerical approximation of self-consistent Vlasov models for low-frequency electromagnetic phenomena", Intern. Journ. of Applied Math. and Comput. Sciences 17 (3) (2007) 1-20

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C. Bardos, I. Catto, N.J. Mauser and S. Trabelsi, "Sufficient condition for the global in time well-posedness of the MCTDHF equations", Applied Math. Letters 22 (2009) 147-152

C. Bardos and N.J. Mauser, "One particle equations for many particle quantum systems : MCTDHF equations", to appear in Quarterly Applied Math. (2009)

N.J. Mauser and S. Trabelsi, "L^2 Analysis of the Time Dependent Multi Configuration Hartree Fock equations", submitted (2009)

C. Bardos, I. Catto, N.J. Mauser and S. Trabelsi, "Setting and Analysis of the Time Dependent Multi Configuration Hartree Fock equations", submitted (2009)

Research Partner / National Partner
Prof. Univ. Doz. Mag. Dr.
Armin Scrinzi

Scientific CV of Armin Scrinzi

Personal Data

Date of birth: 24. 6. 1959

Place of birth: Klagenfurt, Austria

Nationality: Austria

University Education

1978-1985: Master (mathematical physics), U. of Vienna

1985-1989 Dr. rer. nat. (theoretical physics), U. of Vienna

Career History

1985-1991 Research Assistant at I. f. Medium Energy Physics, Vienna

1987-1988 Quantum Theory Project, U. of Florida, Gainesville, US

1990-1991 Postdoc at Kurtchatov Institute, Moscow

1991-1994 Postdoc at Manne Siegbahn Inst., Stockholm

1994-1997 APART Fellowship: U. Cath. de Louvain, Belgium; U. of Southern California, USA, U. of Innsbruck, Austria

1998-2009 Assistant, Photonics Institute, Vienna U. of Technology

2009- Senior group leader, Wolfgang Pauli Institut, Wien

2009 Call as professor to Ludwig Maximilians University, Munich

Publications

About 80 refereed publications h-factor : 28

Awards

1994-1997 APART Fellowship of the Austrian Academy of Sciences

Research Interests

Attosecond dynamics and measurements

Atoms and molecules in strong external fields

Computational Physics

Mathematical Methods – explicitly correlated calculations, complex scaling, MCTDHF

Key Publications (Last 5 Years)

Xinhua Xie, Armin Scrinzi, Marlene Wickenhauser, Andrius Baltuska, Ingo Barth, and Markus Kitzler, Phys. Rev. Lett. 101, 033901 (2008): Internal momentum states for generating circularly polarized X-ray pulses

G. Jordan and A. Scrinzi, New J. Phys., 10, 025035 (2008): Core-polarization effects in molecular high harmonic generation

M. Kitzler, Xinhua Xie, S. Roither, A. Scrinzi, and A. Baltuska, New J. Phys. 10, 025029 (2008): Angular encoding in attosecond recollision

V. Putz, C. Ede, and A. Scrinzi, Phys. Rev. B 76, 35318 (2007): Photoabsorption of Quantum Dots in Quantum Wells with a Strong Electric Bias Field

Xinhua Xie, M. Wickenhauser, W. Boutu, H. Merdji, P. Salieres, A. Scrinzi, Phys. Rev. A76,

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G. Jordan, J. Caillat, C. Ede, and A. Scrinzi, Journal of Physics B 39 341, (2006): Strong field ionization of linear molecules: a correlated 3-dimensional calculation,

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A. Scrinzi, M. Y. Ivanov, R. Kienberger, and D. Villeneuve, J. Phys. B (Topical Review), 39, R1-R37, (2006): Attosecond physics

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M. Kitzler, J. Zanghellini, Ch. Jungreuthmayer, M. Smits, A. Scrinzi, and T. Brabec, Phys. Rev. A, 70, 041401(R) (2004): Ionization dynamics of extended multi-electron systems

J. Zanghellini, M. Kitzler, T. Brabec, and A. Scrinzi, J. Phys. B: At. Mol. Opt. Phys. 37, 763 (2004): Testing the multi-configuration time-dependent Hartree-Fock method

Vladislav S. Yakovlev and Armin Scrinzi, Phys. Rev. Lett., 91, 153901 (2003): High harmonic imaging of few-cycle laser pulses.

O. Smirnova, V. S. Yakovlev, and A. Scrinzi, Phys. Rev. Lett. 91, 253001 (2003): Quantum coherence in the time-resolved Auger measurement.

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Cances E, Le Bris C, 1999, Math. Mod. and Meth. in App. Sci. 9, 963. "On the time-dependent Hartree-Fock equations coupled with a classical nuclear dynamics"

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Drescher M, Hentschel M, Kienberger R, Uiberacker M, Yakovlev V, Scrinzi A, Westerwalbesloh T, Kleineberg U, Heinzmann U, Krausz F, 2002, Nature 419, 803.

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Le Bris C, 1994, Ann. IHP, Anal. Nonlineaire, 171(1), 441. "A general approach for multiconfiguration methods in quantum molecular chemistry"

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Scrinzi A, Ivanov M, Kienberger R, Villeneuve D, J. Phys. B 39, R1-R37, (2006).

Slater J C, 1951, Phys. Rev. 81 (3) , 385 – 390, "A simplification of the Hartree-Fock method"

Wang H and Thoss M, 2003, J. Chem. Phys. 119, 1289.

Zanghellini J, Kitzler M, Fabian C, Brabec T, Scrinzi A, 2003, Laser Physics 13, 1064.

P07: Electronic Structure of Solids, Surfaces and Nanostructures

Project Part Description / Summary

This WIEN2k is a widely used computer program to calculate the electronic structure and properties of solids and surfaces [Blaha01] and is based on the very accurate augmented-plane-wave method. Our method is mainly based on DFT and since the exact functional is unknown, the present functionals use severe approximations. Systematic studies of presently used functionals as well as new developments are vital when one aims to reach "chemical accuracy" in computational materials design.

We plan to:

• Develop and test new semi-local functionals (GGA's and meta-GGA's with improved energetics) or potentials (like mBJLDA for better band gaps) [Haas09a, Tran09].

• Use non-local exchange (Hartree-Fock) and develop/implement/test (modified) hybrid functionals in WIEN2k [Paier06], which should have a broad applicability.

• Apply BSE [Laskowski06] to excited states, in particular for considering core-hole effects in XANES/ELNES spectroscopy. Combine the local MBJLDA potential (or GW [Jiang09]) with BSE (color centers in alkali halides) (P5)

• Collaborate in the development of DFT+DMFT [Held07] for correlated systems (P3).

Furthermore, we plan to develop a module for the calculation of NMR chemical shifts in WIEN2k [Yates07], which together with improved DFT methods could be used to calculate NMR parameters in correlated materials.

The methods developed above will be applied to different materials problems, mostly in cases where standard DFT methods lack sufficient precision, including

• complex magnetic and highly correlated materials, including non-collinear magnetism [Laskowski04], magnetic anisotropies (P12) and exchange interactions [Spiel09]. We also plan to test advanced DFT methods on dilute magnetic semiconductors (P9),

• large-scale problems and nanostructures with several 100 atoms/cell [Laskowski07], where multi-scale methods are highly desirable. We will provide bandstructure calculations for complex graphene-like structures (for tight binding parameters) or silicon nano-wires to investigate how the spin-relaxation time can be increased by valley splitting due to quantum confinement and shear strain [Sverdlov08] (P8). We will also study complex disordered alloys using cluster expansions and Monte Carlo methods (P10),

• predicting the structure of surfaces and interfaces of complex oxides with correlated electrons (in particular oxides used in catalysis); use of genetic algorithms [Oganov08] to find surface structures (P11).

Principal Investigator / Project Part Leader
Ao. Univ. Prof. Dipl.-Ing. Dr.
Peter Blaha

Principal Investigator / Project Part Leader
Ao. Univ. Prof. Dipl.-Ing. Dr.
Peter Blaha

Scientific CV of Peter Blaha

Personal Data

Date of birth: 5.07.1955

Place of birth: Vienna, Austria

Nationality: Austria

University Education

1975-1980: Dipl.-Ing. (Technische Chemie), Technical Univ. (TU) Vienna

1980-1983 Dr. techn., Technical Univ. Vienna

Career History

1980-1992 Assistant, Institut für Techn. Elektrochemie, TU Vienna

1984-1985 Postdoc Louisiana State University, Baton Rouge, USA

1986 Visiting Scientist, Inst.f.Festkörperforschung, KFA Jülich

1988 Guest Prof., University of Florida, Gainesville, USA

1992- A.o.Professor, TU Vienna 1992

1999 Guest Prof., Princeton University, USA

2000 Guest Prof., University Santiago de Compostela, Spain

2005 Guest Prof., Université du Maine, Le Mans, France

Publications

235 refereed publications;

26 invited and plenary lectures in the last 5 years

H-index: 41

Awards

1992 Kardinal Innitzer Award

Research Interests

Density functional theory

Development of the bandstructure code WIEN2k

Physics and chemistry of inorganic materials and their structure and magnetism

Electric field gradients, theoretical spectroscopies

Key Publications (Recent 5 Years)

R. Laskowski, G.K.H. Madsen, P. Blaha, K. Schwarz: "Magnetic structure and electric-field gradients of uranium dioxide: An ab initio study"; Phys. Rev. B 69 ,140408(R) (2004).

I. Sergienko, V. Keppens, M. McGuire, R. Jin, J. He, S. Curnoe, B. Sales, P. Blaha, D.J. Singh, K. Schwarz, D. Mandrus: "Metallic "Ferroelectricity" in the Pyrochlore Cd2Re2O7";

Phys. Rev. Lett. 92, 065501 (2004).

F. Tran, P. Blaha, K. Schwarz, P. Novak: "Hybrid exchange-correlation energy functionals for strongly correlated electrons: Applications to transition-metal monoxides"; Phys. Rev. B 74, 155108 (2006).

R. Laskowski, P. Blaha, T. Gallauner, K. Schwarz: "Single-Layer Model of the Hexagonal Boron Nitride nanomesh on the Rh(111) surface"; Phys.Rev. Lett., 98, 106802 (2007).

F. Tran, R. Laskowski, P. Blaha, K. Schwarz: "Performance on molecules, surfaces, and solids of the Wu-Cohen GGA exchange-correlation energy functional"; Phys. Rev. B 75, 115131 (2007).

S. Berner, M. Corso, R. Widmer, O. Groening, R. Laskowski, P. Blaha, K. Schwarz, A. Goriachko, H. Over, S. Gsell, M. Schreck, H. Sachdev, T. Greber, J. Osterwalder: "Boron Nitride Nanomesh: Functionality from a Corrugated Monolayer"; Ang. Chemie-Int.Edit. 46, 5115 (2007).

J.M. Perez-Mato, L. Elcoro, V. Petricek, H. Katzke, P. Blaha: "Composite Behavior and Multidegeneracy in High-Pressure Phases of Cs and Rb"; Phys. Rev. Lett. 99, 025502 (2007).

M. Body, C. Legein, J. Buzare, G. Silly, P. Blaha, C. Martineau, F. Calvayrac: "Advances in Structural Analysis of Fluoroaluminates Using DFT Calculations of 27Al Electric Field Gradients"; J. Phys. Chem. A 111, 11873 (2007).

H. Dill, J. Lobo-Checa, R. Laskowski, P. Blaha, S. Berner, J. Osterwalder, T. Greber: "Surface Trapping of Atoms and Molecules with Dipole Rings"; Science 319, 1824 (2008).

R. Laskowski, N. Christensen, P. Blaha, B. Palanivel: "Strong excitonic effects in CuAlO2 delafossite transparent conductive oxides"; Physical Review B, 79 (2009), 165209.

C. Spiel, P. Blaha, K. Schwarz: "Density functional calculations on the charge-ordered and valence-mixed modification of YBaFe2O5"; Physical Review B, 79 (2009), 115123.

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P. Haas, F. Tran, P. Blaha: "Calculation of the lattice constant of solids with semilocal functionals"; Physical Review B 79 (2009), 085104; ibid 209902(E)

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P09: Complex Magnetic Structures

Project Part Description / Summary

The application of magnetically doped semiconductors in opto-electronic and spin-electronic devices as well as in quantum computing will have a tremendous scientific and technological importance for the future years. The aim of our project is thus to understand and to predict new materials and novel phenomena for nanomagnetism and spinelectronics. Our approach relies on calculations of the electronic and magnetic structure based on the density functional formalism, which is well suited for a realistic description of the materials and properties involved. Our calculations of the magnetic properties will allow to identify the relevant exchange mechanisms (Zener p-d- exchange, double exchange, super exchange) and the interaction between magnetic moment formation and the electronic structure of the host lattice. Our study also includes the determination of the type of magnetic order, FM, AFM etc. and possible non-collinear magnetic states. Magnetic ordering temperatures, which are of central importance for the application, will mostly be determined from calculations of the exchange parameters. Our investigation will cover p- and transition-element doped II/VI semiconductors like CdS, and ZnO, III/V-systems like GaN and InSb as well as doped graphene. The second important part of our research will investigate magnetism in doped perovskites. Starting from systems like SrTiO3 and BaTiO3 we will study hole doping by replacing oxygen by p-elements from the left site of the main group elements (N,C,P,Si,Al etc.), which will form magnetic moments interacting via the introduced holes. Also for these systems we will study the exchange mechanism. The introduction of magnetic moments in ferroelectric materials could provide a new route towards materials with a strong coupling between magnetic and electric polarization (multiferroics).

Principal Investigator / Project Part Leader
Ao. Univ. Prof. Dipl.-Ing. Dr.
Peter Mohn

Research Partner / National Partner
Ao. Univ. Prof. Dipl.-Ing. Dr.
Josef Redinger

Principal Investigator / Project Part Leader
Ao. Univ. Prof. Dipl.-Ing. Dr.
Peter Mohn

Scientific CV of Peter Mohn

Personal Data

Date of birth: 10.11.1956

Place of birth: Vienna, Austria

Nationality: Austrian

University Education

1975-1981	Dipl.-Ing. (Technische Physik), Technical Univ. (TU) Vienna
1981-1984	Dr. Techn., Technical Univ. Vienna

Career History

1981-1998	Assistant, Institut für Techn. Elektrochemie, TU Vienna
1986-1987	Postdoc Imperial College of Science and Technology, London, UK
1993	Visiting Scientist, University of Melbourne, Australia
1994	Visiting Scientist, University of Uppsala, Sweden
1998-	A.o.Professor, Center for Computational Meterials Science, TU Vienna
1998	Professeur invité, CNRS Lab. de Chimie du Solide, Bordeaux, France
2000, 2002-2003	Guest Prof., University of Uppsala, Sweden

Publications

125 refereed publications; 1 Book; 22 invited and plenary lectures, H-factor 23

Research Interests

Density functional theory and beyond,

Magnetic materials, complex magnetic structures, magnetic semiconductors, multiferroics

Physics and chemistry of inorganic materials and their structure and magnetism, QMC,

Quantum mechanical simulation of precipitation hardening, kinetic MC

Key Publications (Recent 5 Years)

Monograph:

P. Mohn, “Magnetism in the Solid State; An Introduction” Springer Series in Solid-State Sciences, Vol. 134, Springer Verlag 2003 (Berlin, Heidelberg, New York); second printing (soft cover) Springer Verlag 2006 (Berlin, Heidelberg, New York)

Articles:

S. Khmelevskyi, I. Turek and P. Mohn, “Large Negative Magnetic Contribution to the Thermal Expansion in Iron-Platinum Alloys: Quantitative Theory of the Invar Effect“, Phys. Rev. Lett. 91, 037201-1-4 (2003).

Raquel Lizárraga, Lars Nordström, Lars Bergqvist, Anders Bergman, Elisabeth Sjöstedt, Peter Mohn and Olle Eriksson, “Conditions for Noncollinear Instabilities of Ferromagnetic Materials“, Phys. Rev. Lett. 93, 107205 (2004).

S. Khmelevskyi, P. Mohn, J. Redinger and M. Weinert, “Magnetism on the surface of the

bulk paramagnetic intermetallic compound YCo2“, Phys. Rev. Lett., 94, 146403 (2005).

L. Udvardi, S. Khmelevskyi, L. Szunyogh, P. Mohn, and P. Weinberger, “Helimagnetism and competition of exchange interactions in novel bulk GMR alloys based on MnAu2“, Phys. Rev. B, 73 104446 (2006).

M. Sieberer, J. Redinger, S. Khmelevskyi, and P. Mohn, “Ferromagnetism in tetrahedrally coordinated compounds of I/II-V elements; ab-initio calculations“, Phys. Rev. B, 73 024404 (2006).

A. V. Ruban, S. Khmelevskyi, P. Mohn, B. Johansson, “Temperature induced longitudinal Spin fluctuations in Fe and Ni“, Phys. Rev. B, 75 054402 (2007)

Yu. S. Dedkov, C. Laubschat, S. Khmelevskyi, J. Redinger, P. Mohn, M. Weinert, “YCo2: Intrinsic Magnetic Surface of a Paramagnetic Bulk Material“, Phys. Rev. Letters, 99, 047204 (2007).

M. Sieberer, J. Redinger, and P. Mohn, “Electronic and magnetic structure of cuprous oxide Cu2O doped with Mn, Fe, Co, and Ni: A density-functional theory study“, Phys. Rev. B, 75 035203 (2007)

S. Khmelevskyi and P. Mohn, “Layered antiferromagnetism with high Neel temperature in the intermetallic compound Mn2Au“, Appl. Phys. Letters, 93 162503 (2008)

T. Khmelevska, S. Khmelevskyi, and P. Mohn, “Magnetism and structural ordering on a bcc lattice in highly magnetostrictive Fe-Ga alloys: a CPA study“, J. Appl. Phys. 103 073911 (2008).

Research Partner / National Partner
Ao. Univ. Prof. Dipl.-Ing. Dr.
Josef Redinger

Scientific CV of Josef Redinger

Personal Data

Date of birth: 06.02.1955

Place of birth: Tulln, Austria

Nationality: Austria

University Education

1973-1978: Dipl.-Ing. (Technische Chemie), Technical Univ. (TU) Vienna

1978-1983 Dr. techn., Technical Univ. Vienna

Career History

1980-1998 Assistant, Institut für Techn. Elektrochemie, TU Vienna

1982 Visiting Scientist, Hahn-Meitner Institut, Berlin

1986-1987 Postdoc Northwestern University, Evanston, USA

1988, 1989 Visiting Scientist, Northwestern University, Evanston, USA

1992, 1993 Visiting Scientist, Inst.f.Elektron.Eigenschaften, KFA Jülich

1998- A.o.Professor, TU Vienna (Venia Docendi 1993)

Publications

107 refereed publications; 12 invited and plenary lectures, H-factor 24

Research Interests

Density functional theory

Development of the FLAPW bandstructure code FLAIR

Physics and chemistry of metals and insulators, surface, interface and magnetic properties

Theoretical spectroscopies, STM and AFM simulations

Key Publications (Recent 5 Years)

C. Deisl, K. Swamy, N. Memmel, E. Bertel, C. Franchini, G. Schneider, J. Redinger, S. Walter, L. Hammer, and K. Heinz: "(3x1)-Br/Pt(110) structure and the charge-density-wave-assisted c(2x2) to (3x1) phase transition"; Phys. Rev. B 69, 195405 (2004).

S. Khmelevskyi, P. Mohn, J. Redinger, and H. Michor: "Electronic structure of the layered diboride dicarbide superconductor YB2C2"; Supercond. Sci. Technol. 18, 422-426, (2005).

S. Khmelevskyi, P. Mohn, J. Redinger, and M. Weinert: "Magnetism on the surface of the bulk paramagnetic intermetallic compound YCo2"; Phys. Rev. Lett. 94, 146403 (2005).

M. Sieberer, J. Redinger, S. Khmelevskyi, and P. Mohn: "Ferromagnetism in tetrahedrally coordinated compounds of I/II-V elements: Ab initio calculations"; Phys. Rev. B 73, 024404 (2006).

M. Sieberer, J. Redinger, and P. Mohn: "Electronic and magnetic structure of cuprous oxide Cu2O doped with Mn, Fe, Co, and Ni: A density-functional theory study"; Phys. Rev. B 75, 035203 (2007).

M. Minca, S. Penner, T. Loerting, Z. Zhang, A. Menzel, E. Bertel, R. Zucca, and J. Redinger: "Chemisorption of hydrogen on the missing

row Pt(110)-(1x2) surface"; Topics in Catalysis Vol. 46, 161-167 (2007).

E. Dona, T. Loerting, S. Penner, M. Minca, A. Menzel, E. Bertel, J. Schoiswohl, S. Berkebile, F. P. Netzer, R. Zucca and J. Redinger: "Fluctuations and Phase Separation in a Quasi-One-Dimensional System"; Phys. Rev. Lett. 98, 186101-4 (2007).

Yu. S. Dedkov, C. Laubschat, S. Khmelevskyi, J. Redinger, P. Mohn, and M. Weinert: "YCo2: Intrinsic magnetic surface of a paramagnetic bulk material"; Phys. Rev. Lett. 99, 047204-4 (2007).

P. Lazar, J. Redinger, and R. Podloucky: "Density functional theory study of VN/TiN multilayers"; Phys. Rev. B 76, 174112 (2007).

P. Lazar, R. Podloucky, E. Kozeschnik, and J. Redinger: "Density functional theory study of ternary V-Cr-N compounds"; Phys. Rev. B 78, 134202 (2008).

M. Weinert, G. Schneider, R. Podloucky, and J. Redinger: "FLAPW: Applications and implementations"; J. Phys.: Condens. Matter 21, 084201 (2009).

E. Doná, M. Cordin, C. Deisl, E. Bertel, C. Franchini, R. Zucca and J. Redinger: " Halogen induced corrosion of platinum", J. Am. Chem. Soc., 131, 2827 (2009). Chosen as Research Highlight ("Platinum corrosion: A common layer") by Nature Chemistry, Published online: 20 February 2009, doi:10.1038/nchem.161.

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Blaha P., K. Schwarz, G. K. H. Madsen, D. Kvasnicka and J. Luitz, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties

(Karlheinz Schwarz, Techn. Universität Wien, Austria), 2001. ISBN 3-9501031-1-2

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Hohenberg P. and W. Kohn, 1964 Phys. Rev. 136 864.

Hui Pan, Yuan Ping Feng, Qin Yun Wu, and Zhi Gao Huang, 2008 Phys. Rev. B 77 125211.

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Dietl , Y. Ohno, and K. Ohtan, 2000 Nature (London) 408 944.

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Szunyogh L., B. Ujfalussy, P. Weinberger, 1995 Phys. Rev. B 51 9552.

Turek I., V. Drchal, J. Kudrnovský, M. Šob, P. Weinberger, Electronic Structure of Disordered Alloys, Surfaces and Interfaces (Kluwer, Boston, 1997).

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Weinert M., G. Schneider, R. Podloucky, and J. Redinger, 2009 J. Phys.: Condens. Matter 21, 084201; URL: http://www.uwm.edu/~weinert/flair.html.

Weinberger P., L. Szunyogh, 2000 Comp. Mat. Sci. 17 414.

Zajac M., J. Gosk, M. Kaminska, A. Twardowski, T. Szyszko, and S. Podsiadlo, 2001 Appl. Phys. Lett. 79 2432.

P10: Multi-Scale Simulations of Multi-Component Phases

Project Part Description / Summary

The aim of this project is threefold: (i) Use advanced DFT techniques to explore the physical properties of ordered binary and multi-component compounds, concentrating in this first part of the SFB on intermetallic compounds with technologically interesting properties (such as the Ti-based superelastic-superplastic "gum-metal" alloys). (ii) To combine ab-initio DFT calculations with advanced statistical-mechanical tools for exploring the configuration space of disordered multi-component systems, with the aim to extend the applicability of DFT calculations far beyond the scale accessible to current supercell techniques. Our approach will be based on a Cluster Expansion (CE) strategy, using DFT calculations to derive all relevant effective cluster interactions (ECI) from first principles and for calculating the vibrational frequency spectrum, entropy and free energy. Monte Carlo methods will be used to derive the configurational entropy. This will allow to determine the composition-temperature phase diagram, study temperature-induced structural transformations, and to determine the variation of elastic and plastic properties and of the theoretical tensile and shear strength as a function of temperature and composition. (iii) At even larger length scales, Monte Carlo and kinetic Monte Carlo simulations based on different atomic interaction parameters, diffusional jump frequencies and process parameters derived from DFT calculations combined with CE methods will be used to study the microstructure, concentrating on the incipient formation of precipitates (nucleation) in metastable alloys. As a preliminary step for the long term prospect of applying CE also for oxides, the physical properties of selected oxide compounds with varying oxygen concentration will be studied by hybrid functional methods.

Principal Investigator / Project Part Leader
Ao. Univ. Prof. Dr.
Raimund Podloucky

Research Partner / National Partner
o. Univ. Prof. Dipl.-Ing. Dr.
Jürgen Hafner

Research Partner / National Partner
Univ. Prof. Dipl.-Ing. Dr.
Ernst Kozeschnik

Principal Investigator / Project Part Leader
Ao. Univ. Prof. Dr.
Raimund Podloucky

Scientific CV of Raimund Podloucky

Personal Data

Date of birth: 30.07.1948

Place of birth: Vienna, Austria

Nationality: Austria

University education

1967-1975 Dr. phil. (Physics and Mathematics at the University of Vienna)

Career History

1978-1979	Research Scientist, IFF Jülich, Germany
1979-1981	PostDoc., Techn. Univ. Vienna
1981-1982	Research Scientist, Imperial Coll. London, UK
1982-1984	PostDoc., Techn. Univ. Vienna
1984-1986	Research Associate, Northwest. Univ., Evanston, USA
1985	Habilitation: Physical Chemistry, Univ. Vienna
1986-	Permanent position at Inst. Phys. Chemistry, Univ. Vienna
1989	A.o. Univ. Prof

Publications

About 140 refereed publications, 2 book articles, about 20 invited lectures, H-factor 25

Awards

1988 Felix-von-Kuschenitz Award, Austrian Academy of Sciences

Editor

2002-2007	Co-editor of Europhysics Letters (EPL)
2007-	Associate Editor of (EPL)
2008-	Editor of European Physics Journal B

Research Interests

Density functional theory applications to materials properties, phase stabilities, alloy properties, ab initio study of surfaces and interfaces, intermetallics and oxides, mechanical and elastic properties of crystalline solids, magnetic and vibrational properties

Key Publications (Recent 5 Years)

Book Article:

S. Müller, W. Wolf, and R. Podloucky," Ab-Initio Methods and Applications", Alloy Physics: A comprehensive Reference. Ed. Wolfgang Pfeiler, WILEY-VCH Verlag, Weinheim (2007). ISBN: 978-3-527-31321-1

Journal Articles:

C. Franchini, V. Bayer, R. Podloucky, J. Paier, and G. Kresse, "Density functional theory study of MnO by an hybrid functional approach", Phys. Rev. B 72, 045132 (2005).

V. Bayer, C. Franchini, and R. Podloucky, "Ab-initio study of the structural, electronic, and magnetic properties of MnO(100) and MnO(110)", Phys. Rev. B 75, 035404 (2007).

P. Lazar and R. Podloucky, "Ab initio study of tension shear coupling in NiAl", Phys. Rev. B 75, 024112 (2007).

F. Allegretti, C. Franchini, V. Bayer, M. Leitner, G. Parteder ,B. Xu, A. Fleming, M.G. Ramsey, R. Podloucky, S. Surnev, and F.P. Netzer, "Epitaxial stabilization of MnO(111) overlayers on a Pd(100) surface", Phys. Rev. B 75, 224120 (2007):

Xing-Qiu Chen, W. Wolf, P. Rogl, and R. Podloucky, "Structural, magnetic, vibrational and thermodynamic properties of the Laves-phase compound HfMn2", Phys. Rev. B 76, 014424 (2007).

E. Bauer, A. Grytsiv, Xing-Qiu Chen, N. Melnychenko-Koblyuk, G. Hilscher, H.Kaldarar, H. Michor, E. Royanian, G. Giester, M. Rotter, R. Podloucky, and P.Rogl, "Superconductivity in Novel Ge-Based Skutterudites:{Ba,Sr}Pt4Ge12", Phys. Rev. Letters 99, 217001 (2007).

Markus Stöhr, Raimund Podloucky, Martin Gabl, Norbert Memmel, Erminald Bertel, "Combined ab-initio and LEED-I/V study of submonolayer adsorption of In on W(110)", Phys. Rev. B 76, 195449 (2007).

P. Lazar, R. Podloucky, E. Kozeschnik, and J. Redinger, "Density functional theory study of ternary V-Cr-N compounds", Phys. Rev. B 78, 134202 (2008).

P. Lazar and R. Podloucky, "Cleavage fracture of a crystal: Density functional theory calculations based on a model which includes structural relaxations", Phys. Rev. B 78, 104114 (2008).

C. Franchini, R. Podloucky, F. Allegretti, F. Li, G. Parteder, S. Surnev, and F. P. Netzer, "Structural and vibrational properties of two-dimensional MnxOy layers on Pd(100): Experiments and density functional theory calculations", Phys. Rev. B 79, 035420 (2009). (Editor's Suggestion)

M. Stöhr, R. Podloucky, and S. Müller, "Ab initio phase diagram of oxygen adsorption on W(110)", J. Phys.: Condens. Matter 21, 134017 (2009).

F. Li, G. Parteder, F. Allegretti, C. Franchini, R. Podloucky, S. Surnev, F.P. Netzer, "Two-dimensional manganese oxide nanolayers on Pd(100): Surface phase diagram". J. Phys.: Condens. Matter 21, 134008 (2009).

T. Kawakami, Y. Tsujimoto, H. Kageyama, Xing-Qiu Chen, C.L. Fu, C. Tassel, A. Kitada, S. Suto, K. Hirama, Y. Sekiya, Y. Makino, T. Okada, N. Hayashi, K. Yoshimura, S. Nasu, R. Podloucky, and M. Takano, "Spin transition in a four-fold coordinated iron oxide", Nature Chem., accepted (2009).

C. Franchini, G. Kresse, and R. Podloucky, "Polaronic hole trapping in BaBiO3", Phys. Rev. Letters 120, 25640 (2009).

Research Partner / National Partner
o. Univ. Prof. Dipl.-Ing. Dr.
Jürgen Hafner

Scientific CV of Jürgen Hafner

Personal Data

Date of birth: 24.7.1945

Place of birth: Lunz am See, Austria

Nationality: Austria

University Education

1964-1973: Dipl.Ing. Dr. techn. Technische Universität Wien

Career History

1971-75 Research Assistant, Inst. Theoret. Physik, TU Wien

1975-79 Research Associate, MPI Solid State Sciences, Stuttgart

1977 Habilitation, TU Wien

1979-81 Dozent, Inst. Theoret. Physik, TU Wien

1981 Senior Visiting Scientist, Univ. Cambridge

1982-98 Professor, Inst. Theoret. Phys., TU Wien

1983 Professeur Invite, INPG Grenoble

1985 Guest Scientist, Univ. Göttingen

1985 Guest Scientist, Kernforschungszentrum Karlsruhe

1989 Senior Visiting Scientist, Univ. Cambridge

1989 Visiting Fellow, Jap. Soc. Promotion of Science

1998 - Professor, Universität Wien

2005 Professeur Invite, Univ. Paris VI

Publications

About 550 publications in peer reviewed journals, 20 monographs or reviews, 1 book

H-factor 58

Awards

1973 Krafft-Medal, Technische Universität Wien

1979 Ludwig Boltzmann Award , Österr. Physikalische Gesellschaft

1981 Kardinal Innitzer Award

1995 Erwin Schrödinger Award, Österr. Akademie der Wissenschaften

Membership in International Scientific Boards

1996-2003 Steering Committee Research Consortium ''Ab-initio MD applied to Catalysis"

2003-2007 Steering Committee ESF Research Programme ' 'Towards Atomistic Materials Design"

2002-2006 Coordinator Marie-Curie Training Site "Computational Materials Science"

1996-2002 Commission on the Structure and Dynamics of Condensed Matter (C10), IUPAP

2002-2008 Commission on Computational Physics (C20), IUPAP

1990-	Editorial Board, Journal of Non-Crystalline Solids
1995-2001	Co-Editor, Europhysics Letters
2002-2005	Editorial Board, Europhysics Letters
1999-	Editorial Board, Computational Materials Science
2000-2006	Executive Board, Journal of Physics: Condensed Matter

Research Interests

Application of density functional theory to materials science: intermetallic compounds (structure, stability, dynamics, mechanical properties), quasicrystals (structural and electronic properties), magnetism and magnetic materials (ultrathin layers, nanowires, clusters),

surface science and catalysis (catalysis by metals, acid-based catalysis in zeolites and related materials).

Key Publications (Recent 5 Years)

J. Hafner, C. Wolverton, G. Ceder: "Towards atomistic materials design: The impact of DFT calculations on materials research", MRS Bulletion 31, 659 (2006).

M. Krajci , J. Hafner: "Ab-initio studies of quasicrystalline surfaces", in „Quasicrystals", ed. by

T. Fujiwara and Y. Ishii, Handbook of Metal Physics, vol.9, p. 313 (Elsevier 2008).

T. Waitz, D. Spisak, J. Hafner, and H.P. Karnthaler: Nanocrystallinity causing an unexpected martensitic transformation path in NiTi, Europhys. Lett. 71, 98-103 (2005).

J. Hafner, L. Benco, T. Bucko: „Acid-based catalysis in zeolites investigated by density-functional methods", Topics in Catalysis 37, 41 (2006).

S. Dennler and J. Hafner: "A first-principles study of lattice dynamics and diffusion in DO3-type Fe3Si", Phys. Rev. B 73 ,174303/1-14 (2006).

M. Jahnatek, M. Krajci, J. Hafner: "The response of trialuminides to [110] uniaxial loading: Ab-initio study for Al3(Sc,Ti,V)", Phys. Rev. B 76, 014110 (2007).

M.Jahnatek, M. Krajci, J. Hafner: " Interatomic bonds and tensile anisotropy of trialuminides in the elastic limit: A density-functional study for Al3(Sc,Ti, V)", Philos. Mag. 87, 1769 (2007).

D. Spisak, J. Hafner: "The structure and stability of the low-index surfaces of Fe3Si: Ab-initio density-functional investigations", Phys. Rev. B 75, 195411 (2007). Also Virtual Journal of Nanoscale Science and Technology (21 May 2007).

S. Dennler, M. C. Frommen, M.J. Casanove, G. Pastor, J. Morillo, J. Hafner: "Towards atomic-scale materials design: A theoretical investigation of magnetic nanoparticles and ultrathin films", Microelectronics Journal 39, 184 (2008).

M. Krajci, J. Hafner: "Semiconducting Al—transition-metal alloys", in "The Science of Complex Alloy Phases", ed. by T. B. Massalski and P.E.A. Turchi (The Mineral, Metals and Materials Society, Warranedale, PA, 2005), p. 251.

Chao-Hao Hu, A. R. Oganov, Y. M. Wang, H. Y. Zhou, A. Lyakhov, and J. Hafner:"Crystal structure prediction of LiBeH3 using ab-initio total-energy calculations and evolutionary algorithms", J. Chem. Phys. 129, 234105/1-12 (2008)

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beyond", J. Computat. Chem. 29, 2044-78 (2008)

M. Jahnatek, J. Hafner, and M. Krajci: "Shear deformation, ideal strength, and stacking fault formation of fcc metals: A density-functionals study of Al and Cu", Phys. Rev. B 79, 224103/1-17 (2009)

Research Partner / National Partner
Univ. Prof. Dipl.-Ing. Dr.
Ernst Kozeschnik

Scientific CV of Ernst Kozeschnik

Personal Data

Date of birth: 15.01.1966

Place of birth: Leoben, Austria

Nationality: Austria

University Education

1984-1997 Dipl.-Ing. Technical Physics and Dr. techn. (Mechanical Engineering) at the Graz University of Technology

Career History

1998 – 1999 Visiting Scientist, Oak Ridge National Laboratory, Oak Ridge, TN, USA, (Erwin-Schrödinger Scholarship)

1999 – 2004 PostDoc., Assistant Professor, Graz Univ. of Technology

2005 Habilitation: Materials Science, Graz Univ. of Technology

2005-2008 Permanent position at Inst. Materials Science and Technology, Graz Univ. of Technology

2008 Univ. Prof. for "Materials Technology", Vienna Univ. of Technology

Publications

About 100 refereed publications, 2 book editors, about 15 invited lectures, H-factor 8

Awards

2005 'Prof. Koichi Masubuchi Award', of the American Welding Society

2008 'Josef Krainer Würdigungspreis 2008', Province of Styria, Austria.

Research Interests

Phase transformations, Computational microstructure evolution, Continuums modelling of precipitation, atomistic simulations of nucleation, Monte Carlo and Kinetic Monte Carlo, Multi-scale modelling (DFT->CE->(K)MC) of precipitation, multi-component multi-phase systems, diffusion.

Key Publications (Recent 5 Years)

Book Chapters:

"Computational Materials Science - An Introduction to Computational Microstructure Evolution of Polycrystalline Materials", Koenraad G. F. Janssens, Dierk Raabe, Ernst Kozeschnik, Mark A. Miodownik, Britta Nestler, Elsevier Publishing, ISBN 978-0-12-369468-3, 2007, chapter 2 (Thermodynamic basis of phase transformations), chapter 5 (Modeling solid-state diffusion) and chapter 6 (Modeling precipitation as a sharp-interface phase transformation).

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J. Svoboda, E. Gamsjäger, F. D. Fischer, E. Kozeschnik: „Modeling of kinetics of diffusive phase transformation in binary systems with multiple stoichiometric phases“, J. Phase Equil. Diff., 27 (6), 2006, 622-628.

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M. Maalekian, E. Kozeschnik, S. Chatterjee and H. K. D. H. Bhadeshia: „Mechanical Stabilisation of Eutectoid Steel“, Mater. Sci. Techn., 23 (5), 2007, 610-612.

E. Kozeschnik, I. Holzer and B. Sonderegger: „On the potential for improving equilibrium thermodynamic databases with kinetic simulations“, J. Phase Equil. Diff., 28 (1), 2007, 64-71.

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J. Zenisek, J. Svoboda, E. Kozeschnik and F.D. Fischer: „A combined cluster dynamics / kinetic Monte Carlo model for precipitate nucleation in interstitial / substitution alloys“, Modelling Simul. Mater. Sci. Eng., 16 (2008) 075005.

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P11: Nucleation and Self-Assembly in Soft Matter Systems: From the Molecular to the Mesoscopic Scale

Project Part Description / Summary

This subproject is devoted to the development and application of computational methods to bridge length and time scales as they occur, for instance, in the self-assembly of colloidal suspensions. Such soft matter systems now offer exciting new possibilities to study fundamental condensed matter phenomena ranging from melting and freezing [Zahn 1999, Gasser 2001] and the dynamics of glasses [Nugent 2007] to the properties of defects in crystals [Shall 2004, Lechner 2009]. In contrast to their molecular counterparts, these materials can be probed and manipulated with unprecedented "atomic" resolution [Prasad 2007], providing a complete picture of how macroscopic materials properties arise from the underlying microscopic processes. The interactions between the particles can be controlled and tuned to a large degree making it possible to create novel materials that self-assemble into structures of increasing complexity.

One of the key-challenges in the theory and simulation of self-assembly in soft matter is to establish a link between a microscopically resolved picture of the constituent particles and the macroscopic properties of the system. This task is considerably complicated by the vast range of time and length scales characterizing the highly complex self-assembly processes. The chief aim of this subproject is to develop and apply powerful statistical-mechanics-based computational techniques to cope with these problems. Among these methods are genetic algorithm based optimization techniques [Gottwald 2005] and coarse graining methods [Mladek 2008] as well as transition path sampling [Dellago 2002, Dellago 2008] designed to bridge length and time scales, respectively. Focusing on colloidal suspensions as application, we will address questions ranging from the determination of effective interactions governing phase behavior over the identification of self-assembly scenarios to a detailed, time-resolved investigation of the self-assembly process itself. To assess our theoretical approaches we plan a close cooperation with the experimental group of Dr. E. Eiser (Cavendish Laboratory, Cambridge) focused on the self-assembly of DNA-functionalized colloids.

The computational techniques developed and enhanced in this subproject will also serve to address similar space and time scale issues arising in other subprojects of this SFB. While transition path sampling and/or other rare event methods will be applied in the simulations of photochemical processes (P5), precipitation in alloys (P10) and magnetic reversal processes (P12), genetic algorithms and other tools to explore rugged energy landscapes will serve to study the structure of complex oxides (P7). This methodological bridge will stimulate intense interactions between the respective groups.

Principal Investigator / Project Part Leader
Univ. Prof. Mag. Dr.
Christoph Dellago

Research Partner / National Partner
Ao. Univ. Prof. Dipl.-Ing. Dr.
Gerhard Kahl

Principal Investigator / Project Part Leader
Univ. Prof. Mag. Dr.
Christoph Dellago

Scientific CV of Christoph Dellago

Personal Data

Date of birth: 11. 04. 1965

Place of birth: Bozen, Italy

Nationality: Italian

University Education

1985-1991 Mag. (Physics), University of Vienna

1992-1996 Dr. (Physics), University of Vienna

Career History

1990-1993 Software developer, SIEMENS AG, Vienna, Austria

1993-1996 Research Assistant, Inst. f. Experimental Physics, Univ. of Vienna

1996-1999 Postdoc, Dept. of Chemistry, Univ. of California at Berkeley, Berkeley, CA, USA

1999-2003 Assistant Professor, Dept. of Chemistry, Univ. of Rochester, Rochester, NY, USA

2003- Full Professor, Computational Physics, Faculty of Physics, Univ. of Vienna

2008-2009 Vice-Dean of the Faculty of Physics, Univ. of Vienna

2009 Dean of the Faculty of Physics, Univ. of Vienna

Publications

About 90 refereed publications, H-factor 25

About 30 invited lectures at international conferences

Awards

1996 Schrödinger Fellowship of the Austrian Science Foundation FWF

1997 Förderpreis der Stiftung zur Förderung junger Südtiroler im Ausland

2005 The Raymond and Beverly Sackler Prize awarded by Tel Aviv University

Research Interests

Simulation methods for rare events

Non-equilibrium statistical mechanics

Soft matter

Chemical reaction dynamics

Proton transfer in aqueous media

Structural and morphological transitions in nanoparticles

Molecular dynamics and Monte Carlo simulation

Key Publications (Recent 5 Years)

W. Lechner and C. Dellago, " Defect interactions in two-dimensional colloidal crystals: vacancy and interstitial strings", Soft Matter, in print (2009).

M. Grünwald and C. Dellago, "Nucleation and growth in structural transformations of nanocrystals", Nano Letters 9, 2099 (2009).

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M. Grünwald, P. L. Geissler, and C. Dellago, "An efficient transition path sampling algorithm for nanoparticles under pressure", J. Chem. Phys. 127, 154718 (2007).

H. Oberhofer, C. Dellago, and S. Boresch, "Single molecule pulling with large time steps", Phys. Rev. E 75, 061106 (2007).

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W. Lechner, H. Oberhofer, C. Dellago, and P. L. Geissler, "Equilibrium free energies from fast-switching simulations with large time steps", J. Chem. Phys. 124, 044113 (2006).

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Y. Wang, S. Teitel, and C. Dellago, "Surface driven bulk reorganization of gold nanorods", Nano Lett. 5, 2174 (2005).

A. Tröster and C. Dellago, "Wang-Landau Sampling with Self-adaptive Range", Phys. Rev. E 71, 066705 (2005).

Y. Wang, S. Teitel, and C. Dellago, "Melting and equilibrium shape of icosahedral gold nanoparticles", Chem. Phys. Lett. 394, 257 (2004).

C. Dellago and P. G. Bolhuis, "Activation energies from transition path sampling simulations", Molecular Simulation 30, 795 (2004).

W. Zhuang and C. Dellago, "Dissociation of hydrogen chloride and proton transfer in liquid glycerol: an ab initio molecular dynamics study ", J. Phys. Chem. B 108, 19647 (2004).

Research Partner / National Partner
Ao. Univ. Prof. Dipl.-Ing. Dr.
Gerhard Kahl

Scientific CV of Gerhard Kahl

Personal Data

Date of birth: 07.01.1957

Place of birth: Vienna, Austria

Nationality: Austria

University Education

1975-1979 Dipl.-Ing. (Technische Physik), TU Wien

1980-1983 PhD TU Vienna; 1984; Dr. techn.

Career History

1980-1986 Assistant, Institut für Theoretische Physik, TU Wien

1986-1987 Post-doc at the Université Pierre et Marie Curie, Paris, France

1988 Habilitation in 'Condensed Matter Theory'

1997- Associate Professor, Institut für Theoretische Physik, TU Wien

Publications

About 125 refereed publications, H-factor 20

About 20 invited lectures at international conferences

Awards

1984 PhD ‚summa cum laude', TU Wien, Austria

1984 'Ludwig Wittgenstein' scholarship of the Österreichische Forschungsgemeinschaft

1986 ‚Erich Schmid' Award, Austrian Academy of Science

1994 'Kardinal Innitzer' prize

Research Interests

All aspects of phase behaviour (in particular self-assembly scenarios) of soft matter systems, based on classical liquid state theory, classical density functional theory, computer simulations, and genetic algorithms; particular emphasis on colloidal dispersions, establishing a link between a monomer resolved picture of the particles and the macroscopic systems.

Key Publications (Recent 5 Years)

D. Gottwald, C.N. Likos, G. Kahl, and H. Löwen, "Phase behaviour of ionic microgels", Phys. Rev. Lett. 92, 068301-1 - 68301-4 (2004); also published in: Virtual Journal of Nanoscale Science & Technology (23.2.2004).

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J. Köfinger, N.B. Wilding, and G. Kahl, "Phase behaviour of a symmetrical binary fluid mixture", J. Chem. Phys. 125, 234503-1 - 234503-15 (2006).

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Nugent C R, Edmond K V, Patel H N, and Weeks E R, 2007, Phys. Rev. Lett. 99, 025702.

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P12: Multi-Scale Simulations of Magnetic Nanostructures

Project Part Description / Summary

The ability to calculate the long-time thermal stability of magnetic nanostructures is the basis of the design of any storage component such as hard disk drives, magnetic random access memories and advanced race track memories [Parkin 2008]. Micromagnetics is a perfect tool to study magnetization dynamics on a length-scale of nanometers and typical time scales of nanoseconds. However, the important question of the thermal stability on a time scale of years goes beyond the methods of standard micromagnetics. Within the project we aim to develop a multi-scale micromagnetic approach that is suitable (i) to bridge the gap between the picosecond time scale of precessional motion and that of magnetic reversal processes of years, and (ii) to combine ab-initio simulations of magnetic structures with multiscale simulations for the design of novel structures and devices. We aim to achieve the first goal by applying Transition Path Sampling (TPS) [Dellago 1998], a computational method for finding mechanism and rate constants of processes dominated by rare events. In contrast to other methods such as transition state theory [Hänggi 1990], TPS is the ideal tool for the simulation of granular magnetic recording films, where multiple energy barriers between the initial state and the final state are expected. Within the project we will combine the micromagnetic code (FEMME) developed at the Institute of Solid State Physics with the TPS code of C. Dellago (P11). The bounce algorithm is used to construct transitions paths that act as an input for TPS. In order to speed up the computational time the super linear Kronecker approximation is implemented in order to solve the strayfield problem.

In order to reach the second goal of bridging the length-scales, the results from atomistic ab-initio simulations (P7) such as surface anisotropy constants and magnetostrictive constants, material properties at the interface between magnetic domains etc. are combined with micromagnetic simulations. In particular, it is aimed to combine a strayfield energy in the ab-initio codes that follows from micromagnetic simulations. By taking into account the domains of magnetic structures it is expected that the ground state energies can be calculated more accurately. Prediction of the critical thickness when a perpendicular magnetization rotates inplane will be possible due to the inclusion of realistic demagnetization fields. In close cooperation with P7 a magnetostrictive term is implemented in micromagnetics. In order to simulate a macroscopic sensor device the limitations of micromagnetics have to be overcome. This is done by combine a hybrid finite element/boundary element strayfield calculation method with methods of Maxwell solver.

Principal Investigator / Project Part Leader
Privatdoz. Dipl.-Ing. Dr.
Dieter Süss

Research Partner / National Partner
Univ. Prof. FH-Prof. Dipl.-Ing. Dr.
Thomas Schrefl

Principal Investigator / Project Part Leader
Privatdoz. Dipl.-Ing. Dr.
Dieter Süss

Scientific CV of Dieter Süss

Personal Data

Date of birth: 15.12.1975

Place of birth: Vienna, Austria

Nationality: Austria

University Education

1994-1999:	Dipl.-Ing. (Technische Physik), Technical Univ. (TU) Vienna
2000-2002	Dr. techn., Technical Univ. Vienna
2007	Habilitation (Computational Material Science)

Career History

2003 – 2008	Post-Doc at the University of Technology
2005 (June-July)	Hitachi Global Storage System, San Jose, USA
2006 (July-September)	Consultant, Komag Inc, San Jose USA
2008 -	Institute of Solid State physics (Project Leader)

Publications

105 refereed publications (H-factor 14); 9 book chapters, 10 invited talks, 5 plenary talks and keynote lectures in the last 3 years, one pending patent (Multilayer Exchange Spring Recording Media) Application Number 11/424,859

Research Interests

Micromagnetics

Spin electronics

Spin dynamamics

Magnetic storage applications

Key Publications

D. Suess, M Kirschner, T. Schrefl, J. Fidler, R.L. Stamps, T. Schrefl, J.V. Kim, "Exchange bias of polycrystalline antiferromagnets with perfectly compensated interface", Phys. Rev.B 67, 54419 (2003).

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O. Ertl, G. Hrkac, D. Suess, M. Kirschner, F. Dorfbauer, J. Fidler, and T. Schrefl, "Multiscale micromagnetic simulation of giant magnetoresistance read heads," J. Appl. Phys. 99, 08S303 (2006).

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F. Dorfbauer, T. Schrefl, M. Kirschner, G. Hrkac, D. Suess, O. Ertl, and J. Fidler, "Nanostructure calculation of CoAg core-

shell clusters," J. Appl. Phys. 99, 08G706 (2006).

D. Suess, S. Eder, J. Lee, R. Dittrich, J. Fidler, J. W. Harrell, T. Schrefl, G. Hrkac, M. Schabes, N. Supper, and A. Berger, "Reliability of Sharrocks equation for exchange spring bilayers," Phys. Rev. B, 75, 174430 (2007).

D. Suess, J. Fidler, G. Zimanyi, T. Schrefl, and P. Visscher, "Thermal stability of graded exchange spring media under the influence of external fields", Appl. Phys. Lett. 92, 173111 (2008).

G. Hrkac, T. Schrefl, S. Bance, D. Allwood, A. Goncharov, J. Dean, and D. Suess, "Mutual phase locking in high-frequency microwave nano-oscillators as a function of field angle," J. Magn. Magn. Mater., 320, L111 (2008).

J. Dean, M. A. Bashir, A. Goncharov, G. Hrkac, S. Bance, T. Schrefl, A. Cazacu, M. Gubbins, R. W. Lamberton, and D. Suess, "Thermally induced adjacent track erasure in exchange spring media," Appl. Phys. Lett. 92, 142505 (2008).

Research Partner / National Partner
Univ. Prof. FH-Prof. Dipl.-Ing. Dr.
Thomas Schrefl

Scientific CV of Thomas Schrefl

Personal Data

Date of birth: 26.3.1965

Place of birth: St. Pölten, Austria

Nationality: Austria

University Education

1983-1991:	Dipl.-Ing. (Technische Physik), Technical Univ. (TU) Vienna
1991-1993	Dr. techn., Technical Univ. Vienna
1999	Habilitation (Computational Physics)

Career History

1995 –1999	Researcher, Institute for Applied and Technical Physics
2001 –2002	Researcher at the IBM Almaden Research Center, CA
2000 –2004	Project Leader, Start Program (Y132-PHY)
2004 -	Professor of functional Materials (University of Sheffield)
2009 -	Dozent FH. St. Pölten

Awards

1999	Start Price of the FWF
2005	Wohlfarth Memorial Lecturer

Publications

186 refereed publications ((H-factor 22); 22 invited reviews and book chapters, 120 invited talks and lectures, 18 plenary talks and keynote lectures

Research Interests

Computersimulations,

magnetic storage,

Spin electronics,

Spin dynamamics,

List of Literature

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Miscellaneous

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Contact Information

For further information, please contact Mr. Seiichi Chikama (Secretary). Thank you in advance.

phone: +43 1 4277 51402
fax: +43 1 4277 9733
e-mail: seiichi.chikama[at]univie.ac.at

Website

http://www.sfb-vicom.at