The IFF Spring School & Computational Materials Physics in Jülich

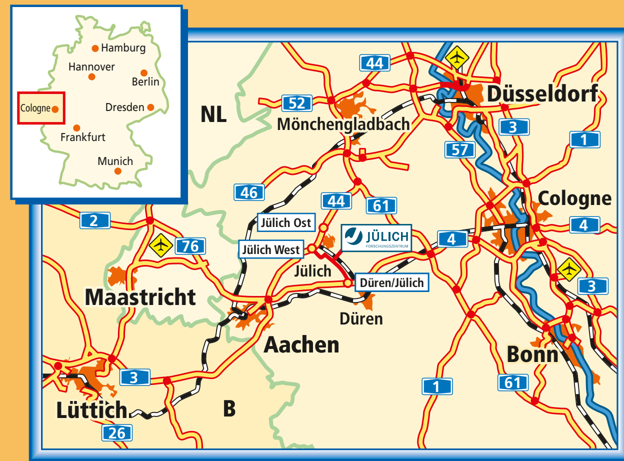
The IFF Spring Schools were first brought into being in 1970 by the "Institut für Festkörperforschung" (IFF). Since then, they have made it possible for students and young scientists to gain a two-week insight into a current topic related to condensed matter physics. In 2011, IFF was dissolved as part of a restructuring process within Forschungszentrum Jülich, and new institutes, namely the "Peter Grünberg Institut" (PGI), the "Jülich Centre for Neutron Science" (JCNS) and the "Institute of Complex Systems" (ICS) were established. Together with the "Institute for Advanced Simulation" (IAS), they will continue to coordinate the IFF Spring Schools. The 45th Spring School 2014 will be organized by PGI-1 / IAS-1 "Quantum Theory of Materials" together with the Theoretical Solid State Physics Group from the RWTH Aachen University.

Forschungszentrum Jülich has a long track record of advancing research in the field of computational materials physics and materials science. At a very early stage, scientists here recognized the importance of computer simulation as a source of knowledge in condensed matter physics. With the advent of peta-flop computing based on new architectural concepts, scientific computing is transforming to simulation sciences. Together with the Jülich Supercomputing Centre (JSC), the German Research School for Simulation Sciences (GRS), established under the umbrella of the Jülich-Aachen Research Alliance (JARA), and the recently founded Institute for Advanced Simulation (IAS), Forschungszentrum Jülich is home to a research triangle where education, different research disciplines together with methodical and technological competences are combined to manage the future challenges in simulation sciences.

The Institute "Quantum Theory of Materials" develops conceptual and computational methods based on density-functional theory. It supports an "ab initio" simulation laboratory. Computational materials science research is established by combining first-principles results with dynamical and statistical methods (molecular dynamics, Monte Carlo). The institute focuses on the analysis and computation of electronic properties of solid-state systems relevant for nanoelectronics (spintronics, nanoionics, complex magnetism, organic molecules) and energy.

The development of quantum many-body methods and their application in model systems of correlated electrons has a long history at the physics department of RWTH Aachen University. Nowadays, the department is split into the institutes of Theory of Statistical Physics and Theoretical Solid State Physics. The research pursued in the former is focused on correlation effects in mesoscopic systems including the rapidly developing field of non-equilibrium phenomena, using renormalization group-based approaches. In the latter, such methods as well as numerical tools (e.g. quantum Monte Carlo) are used to investigate the physics of correlated materials.

How to find us:



Scientific Organization

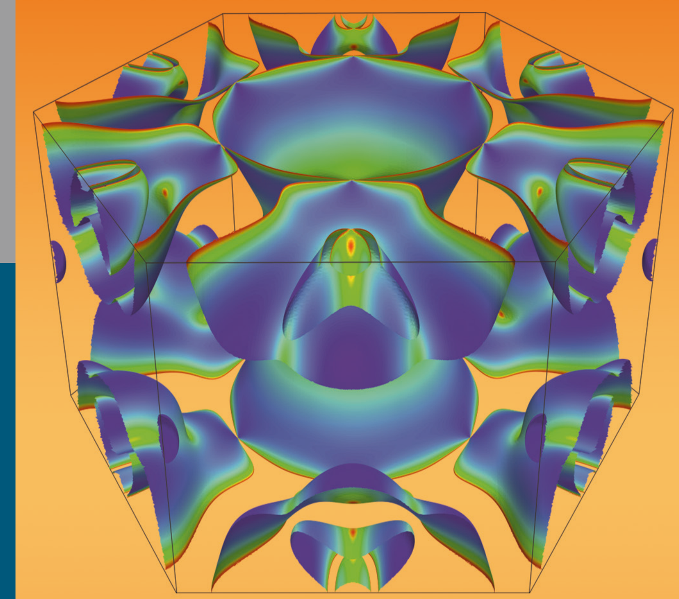
Stefan Blügel
Nicole Helbig
Volker Meden
Daniel Wortmann

School Organization

Michael Beißel
Forschungszentrum Jülich GmbH
Peter Grünberg Institut / Jülich Centre for Neutron Science
52425 Jülich
Germany
Tel: +49 2461 61 1739
Fax: +49 2461 61 2410
Email: springschool@fz-juelich.de

Registration and Further Information
www.iff-springschool.de

The lecture programme, travelling information, and participant card will be sent in due course to all registered participants.



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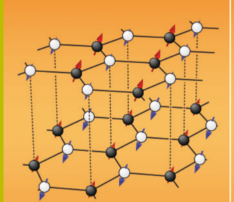

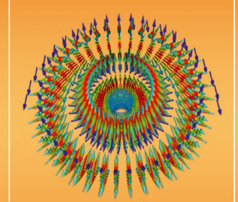

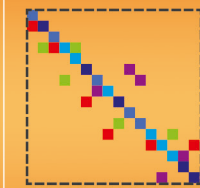

Computing Solids

Models, ab-initio methods and supercomputing

45th IFF Spring School 2014
March 10 – 21, 2014 in Jülich, Germany

JÜLICH
FORSCHUNGSZENTRUM

Overview

Computational materials physics is concerned with the complex interplay of the myriad electrons and atoms in a solid, thereby producing a continuous stream of new and unexpected phenomena and forms of matter. An extreme range of length, time, energy and entropy scales give rise to the complexity of an extremely broad range of solids and associated properties. There are literally hundreds of thousands of solids. Some solids exhibit useful or exotic phases, such as ferroelectricity, magnetism, superconductivity, or take on exotic states of matter such as the heavy fermion state. Other solids exhibit interesting metal to insulator transitions or show transversal, quantum and non-equilibrium transport processes, to mention but a few. Every day, new solids are synthesised or grown and novel properties are discovered. These solids find applications as present and emergent materials with specially-designed functionalities on which technological advances in fields such as information technology, energy harvesting, storage and conversion, material science, chemistry and even biology rest on.

It sounds rather like a miracle, but the formation and stability of all solids and their properties are encoded in the statistical physics and quantum theory of the many electrons in the solid interacting via the Coulomb potential. Therefore, the Schrödinger equation of many electrons provides a fundamental theoretical concept for the understanding of a large variety of quantum phenomena that could be exploited in future technological devices. The exact solution of such a Schrödinger equation for a solid is not in sight. Instead, in the past decades powerful theoretical concepts have been developed that allow effective approximations, aimed at reducing complexity while retaining those ingredients necessary for a reliable description of the physical effects in the system.

The approximations of the quantum many-body problem may be roughly divided into three different classes: wave function based methods, ab-initio density functional approaches, and realistic model Hamiltonians, that are solved in part with sophisticated and highly specialized many-body methods such as renormalization techniques or quantum Monte Carlo.

Due to the length and the time scales of the systems investigated, the complexity of the interactions and the possible degree of non-equilibrium, this field has benefited tremendously from the exponential growth of computer resources, in part with new computer architectures. Adapting existing computer codes or developing new codes for these new infrastructures is an increasingly pressing and demanding topic in any computational based research.

Program

The IFF Spring School 2014 will provide a comprehensive introduction to modern concepts, theories and methods enabling the theoretical description of many-electron systems. The hallmark of this year's school is in the concept of discussing density functional theory type ab-initio approaches as well as specialized many-body techniques for strongly correlated systems emphasizing the new opportunities provided by high-performance computers with advanced architectures. The school links these three aspects to the study of emergent properties of solids and non-equilibrium quantum transport. The guiding principle for the selection of the specialized subjects was their timeliness and the expertise of the scientific institutes involved. The school will start with introductory lectures on the many-electron problem. Basic lectures will introduce the different methodologies but will also bring in cutting edge research in the field. The formulation of realistic model Hamiltonians links density functional theory to the many-body methods. The school will move on to discuss solutions to the many-body problem of model systems, either analytically using renormalization group techniques, or numerically using different computational implementations. The School will then advance to the calculation of different materials and physical effects. One emphasis is the quantum and topological transport properties. The School also includes lectures on computational topics addressing the recent and future advances in computer architecture and technology. These lectures will especially focus on how the computational resources can be exploited for the simulation of complex materials, for example, via parallel programming or how large computing resources change the paradigm of materials research, for example by database oriented material design approaches.

The topics of the lectures cover:

- Density functional theory and methods
- Many-body perturbation theory
- Model Hamiltonians
- Renormalization group techniques
- Berry phase physics and Wannier functions
- Nonequilibrium quantum-transport and open systems
- Application to graphene, magnetic skyrmions, pnictides
- Materials Informatics and Design
- Simulation techniques
- Parallel Computing

The IFF Spring School is organized in close collaboration with universities, research institutions and industry. The School offers around 45 hours of lectures plus discussions as well as the opportunity to visit the participating institutes at the Forschungszentrum Jülich. All lectures will be given in English. Each registered participant will receive a copy of the lecture notes (in English), which contain all the material presented during the school.

General Information

Venue

The IFF-Spring School will take place in the Auditorium of the Forschungszentrum Jülich from March 10 – 21, 2014.

Participation

Participants are expected to have a basic knowledge of condensed matter physics.

Registration Deadline

All participants are asked to register via internet at **www.iff-springschool.de** before January 31, 2014.

Travel Information

A shuttle service will take participants to Forschungszentrum Jülich in the morning and back to their accommodation after the lectures are concluded. The daily transfer is free for all registered participants.

Accommodation, Lunch and Dinner

Low-cost accommodation will be arranged at a youth hostel in Aachen. The accommodation fee of € 360 includes breakfast and dinner. Lunch will be provided at the Forschungszentrum Jülich from Monday to Friday at your own cost.

Arrival: Sunday, March 9, 2014
Begin of lectures: Monday, March 10, 2014
Departure: Friday afternoon, March 21, 2014

Students who have not yet finished their Master's degree can apply for financial support from the Forschungszentrum Jülich to cover part of the accommodation costs. To qualify for this support, valid proof of student status must be supplied. Accommodation for participants from nearby universities can only be provided if there are still places available after the registration deadline

Payment and Cancellation Policy

On completing registration for IFF-Spring School you will receive E-Mail confirmation. Participants who are in need of accommodation at the Youth Hostel will receive an invoice with all relevant information regarding the transfer of the accommodation-fee in due time. Cancellations must be received before March 04, 2014, otherwise a payment of Euro 50 is required.

Hotels in Aachen and Jülich

If you would prefer to stay in a hotel in Aachen or Jülich at your own cost, please contact **springschool@fz-juelich.de** for an accommodation list.