

NIC Winter School 2006

Computational Nanoscience: Do it yourself!

(<http://www.fz-juelich.de/conference/wscn>)

14-26 Februar 2006

Forschungszentrum Juelich, Germany

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Scope and Aim of the School:

This hands-on NIC Winter School focuses on the application of modern electronic structure calculations and dynamical simulation techniques covering aspects of solid state and surface science, chemical reactions and dynamics, as well as the structure and properties of large molecules and clusters. The School will provide a practical introduction to the theory behind and handling of pertinent software packages through practicals and tutorials in small groups using four codes. The full-potential linearized augmented plane wave code FLEUR and the Korringa-Kohn-Rostocker Green function code KKR-GF, the ab initio (Car-Parrinello) molecular dynamics simulation package CPMD, and the highly efficient quantum chemistry code TURBOMOLE. Although very different in concept and application focus, all these codes are well-known prototypical representatives and are used in various supercomputer centres around the world.

This School about "electronic structure at work" is tailored for PhD students and Postdocs with a solid background in basic quantum mechanics coming from physics, chemistry, material science and related disciplines. The School combines lectures in the morning, which elucidate the theoretical concepts and numerical procedures, with practical sessions in the afternoon. Within these practicals, bridges will be built from simple test examples up to realistic research problems. It is the aim of this NIC Winter School that participants gain a broad but nevertheless deep understanding of what state-of-the-art electronic structure methods can currently achieve.

Format of the School:

It is a typical "hands-on-school" with lectures in the morning and tutorials in the afternoon sessions and weekend. We introduce 4 possible representative codes: FLAPW-code FLEUR, KKR-Greenfunction-Code, TURBOMOL-code, Car-Parrinello-code CPMD. Participants have to sign-up for one of them after the 1st day for the afternoon tutorials.

Participants:

The school aims at PhD students and young postdocs. It is limited to 40 participants.

Funding:

I would like to ask for funding from the ESF Psi_k Program to support mostly graduate students in exceptional cases also postdocs of our community in order to encourage their participation. We hope to offer at least 20 scholarships of 350 Euro to cover living expenses and 10 scholarships of 250 Euro for travel expenses. Therefore, we apply for a total amount of 9500 Euro.

We expect that the Forschungszentrum Juelich will contribute 20.000 Euro to cover the expenses of the invited speakers, the publication of the lecture notes, the local infrastructure, transportation between accomodation and laboratory and the computer infrastructure.

Tentative List of Teachers:

G. Bihlmayer (IFF, Juelich)

- Non-Collinear Magnetism, Exchange Parameter and Tc

S. Blügel (IFF, Juelich)

- The FLAPW Method

P.H. Dederichs (IFF, Juelich)

- KKR-GF Method for Impurities, Clusters on Surfaces

N. Doltsinis (Theo. Chemistry, Bochum, Germany)

- Advanced Sampling via Molecular Dynamics

- Time-Dependent DFT

- Molecular Dynamics Beyond the Adiabatic Approx.

Ch. Hättig (INT, Karlsruhe)

- Beyond Hartree-Fock: MP2 and Coupled Cluster Methods

- R.O. Jones (IFF, Juelich)
- Introduction to Density Functional Theory
- On Exchange Correlations Functionals (LDA and GGA)
- B. Körfgen (ZAM, Juelich)
- Parallel Linear Algebra Methods
- St. Kurth (FU-Berlin, Berlin)
- Beyond the Local Density Approximation:
- The Optimized Effective Potential Method and LDA+U
- D. Marx (Theo. Chemistry, Bochum)
- Ab Initio Molecular Dynamics: Car-Parrinello and Born-Oppenheimer
- Ph. Mavropoulos (IFF, Juelich)
- The KKR Green Function Method
- B. Meyer (Theo. Chemistry, Bochum)
- Ab Initio Thermodynamics
- The Pseudo-Potential Plane Wave Approach
- B. Mohr (ZAM, Juelich)
- Introduction to Parallel Computing
- Th. Müller (ZAM, Juelich)
- Basis Sets, Accuracy, and Calibration in Quantum Chemistry
- M. Scheffler (Fritz-Haber-Institut, Berlin)
- Ab initio Electronic Structure Calculations: Status and Challenges
- A. Schindlmayr (IFF, Juelich)
- Many-Particle Perturbation Theory: GW and BSE
- V. Staemmler (Theo. Chemistry, Bochum)
- Introduction to Hartree-Fock and CI Methods
- G. Sutmann (ZAM, Juelich)
- Molecular Dynamics Simulations
- D. Wortmann (IFF, Juelich)
- Ab Initio Transport
- R. Zeller (IFF, Juelich)
- Spin-Polarized DFT Calculations and Magnetism

Preliminary Programme:

Tuesday

- 13:00 - 14:00 Registration
- 14:00 - 14:15 Opening Remarks / Richard Wagner and Organizer
- 14:15 - 15:15 Ab initio Electronic Structure Calculations/ Matthias Scheffler
- 15:15 - 16:15 Introduction to Hartree-Fock and CI Methods/ Volker Staemmler
- 16:15 - 16:45 Coffee
- 16:45 - 17:45 Introduction to Density Functional Theory / Robert O. Jones
- 18:00 - 20:00 Reception and get-together (ZB-Foyer)

Wednesday

- 9:00 - 10:00 The Pseudo-Potential Plane Wave Approach / Bernd Meyer
- 10:00 - 11:00 The FLAPW Method / Stefan Blügel
- 11:00 - 11:30 Coffee
- 11:30 - 12:30 Introduction to Parallel Computing / Bernd Mohr
- 12:30 - 14:00 Lunch
- 14:00 - 15:00 Parallel Linear Algebra Methods / Bernd Körfgen
- 15:00 - 18:00 Practical Session 1: Parallel Linear Algebra
Coffee (ZAM Foyer)

Thursday

- 9:00 - 10:00 The KKR Green Function Method / Phivos Mavropoulos
- 10:00 - 11:00 Basis Sets, Accuracy, ... in Quant. Chem. / Thomas Müller
- 11:00 - 11:30 Coffee
- 11:30 - 12:30 Molecular Dynamics Simulations / Godehard Sutmann
- 12:30 - 14:00 Lunch
- 14:00 - 15:00 Ab Initio MD: CP and Born-Oppenheimer / Dominik Marx
- 15:00 - 18:00 Practical Session 2: Getting Familiar with the Codes
Coffee (ZAM Foyer)

Friday

- 9:00 - 10:00 On Exchange Correlations Functionals / Robert Jones
- 10:00 - 11:00 Spin-Polarized DFT Calculations and Magn./ Rudolf Zeller
- 11:00 - 11:30 Coffee
- 11:30 - 12:30 Ab Initio Thermodynamics / Bernd Meyer
- 12:30 - 14:00 Lunch
- 14:00 - 18:00 Practical Session 3: Determining the Structure of Solids,
Liquids, and Clusters
Coffee (ZAM Foyer)
- 18:00 - 20:00 Poster Session (contribution from participants)

Saturday

- 9:00 - 18:00 Practical Session 4: Pick Your Favored Problem and
Work on it
Catered lunch

Sunday

- 9:00 - 18:00 Excursion

Monday

- 9:00 - 10:00 Beyond HF: MP2 and Coupled Cluster Meth. / Christof Hättig
10:00 - 11:00 Non-Coll. Magnetism: J_{ij} and T_c / Gustav Bihlmayer
11:00 - 11:30 Coffee
11:30 - 12:30 The KKR-GF Method for Impurities + Clusters / Peter H. Dederichs
12:30 - 14:00 Lunch
14:00 - 18:00 Practical Session 5: Computing Properties of Solids,
Liquids, and Clusters
Coffee (ZAM Foyer)

Tuesday

- 9:00 - 10:00 Advanced Sampling via Molecular Dynamics / Nikos Doltsinis
10:00 - 11:00 Time-Dependent DFT / Nikos Doltsinis
11:00 - 11:30 Coffee
11:30 - 12:30 Beyond the LDA: The OEP and LDA+U / Stefan Kurth
12:30 - 14:00 Lunch
14:00 - 18:00 Practical Session 6: Applications "à la Carte"
Coffee (ZAM Foyer)

Wednesday

- 9:00 - 10:00 MD Beyond the Adiabatic Approximation / Nikos Doltsinis
10:00 - 11:00 Ab Initio Transport / Daniel Wortmann
11:00 - 11:30 Coffee
11:30 - 12:30 Many-Particle Perturbation Theory: GW,BSE/ Arno Schindlmayr
12:30 - 12:45 Closing Remarks: Stefan Blügel / Johannes Grotendorst / Dominik Marx
12:30 - 14:00 Lunch