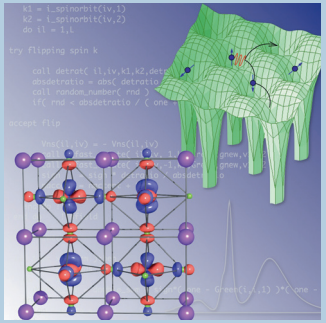
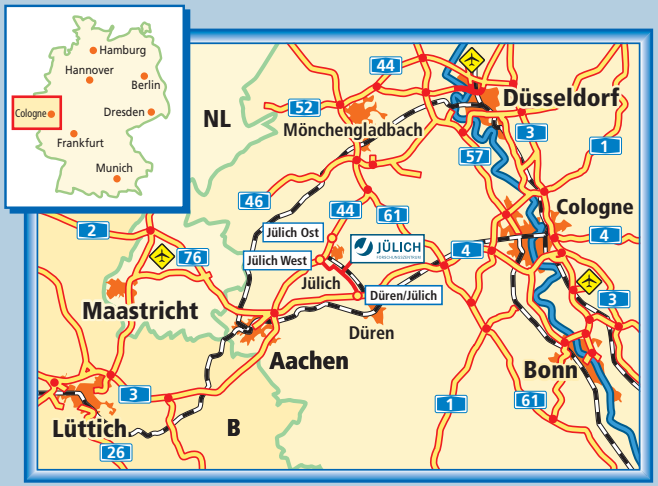


DFG Research Unit FOR 1346

Dynamical Mean-Field Approach
with Predictive Power for
Strongly Correlated Materials

http://www.physik.uni-augsburg.de/for1346

- Fakher Assaad (Würzburg)
- Peter Blöchl (Clausthal)
- Stefan Blügel (Jülich)
- Nils Blümer (Mainz)
- Ralph Claessen (Würzburg)
- Hubert Ebert (München)
- Maurits Haverkort (Stuttgart)
- Karsten Held (Wien)
- Harald Jeschke (Frankfurt)
- Daniel Khomskii (Köln)
- Erik Koch (Jülich)
- Marcus Kollar (Augsburg)
- Georg Kresse (Wien)
- Jan Kuneš (Prag)
- Frank Lechermann (Hamburg)
- Alexander Lichtenstein (Hamburg)
- Jan Minár (München)
- Eva Pavarini (Jülich)
- Michael Potthoff (Hamburg)
- Thomas Pruschke (Göttingen)
- Hao Tjeng (Dresden)
- Alessandro Toschi (Wien)
- Roser Valentí (Frankfurt)
- Dieter Vollhardt (Augsburg)
- Philipp Werner (Zürich)

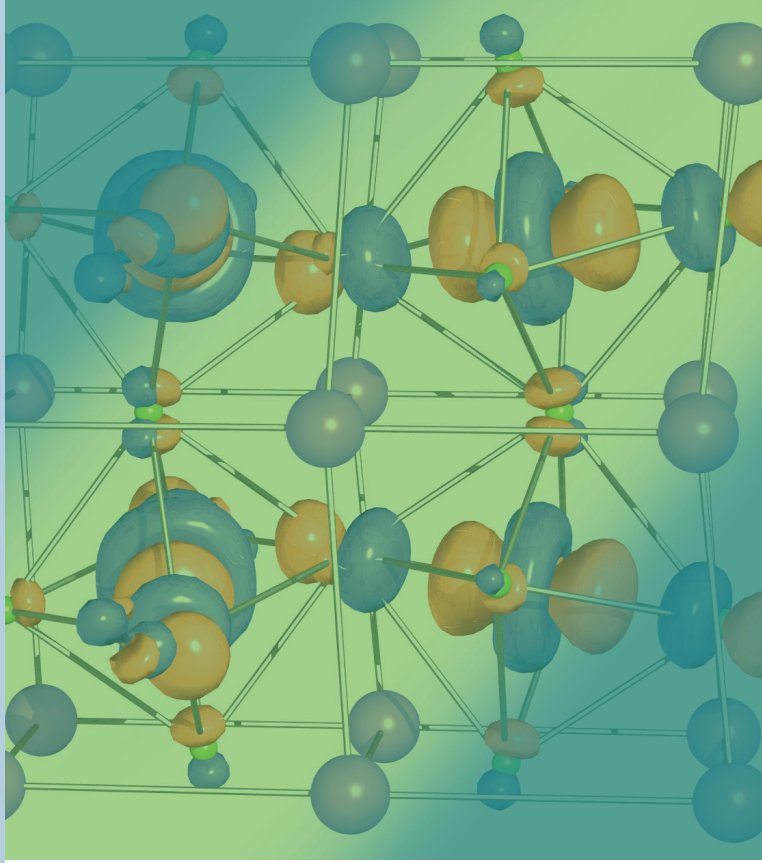


Organizers

Eva Pavarini, Forschungszentrum Jülich
Erik Koch, German Research School, Jülich
Dieter Vollhardt, Universität Augsburg
Alexander Lichtenstein, Universität Hamburg

Further information

Please refer to www2.fz-juelich.de/iff/correl11 for more information and updates. For further questions, please write to correl11@fz-juelich.de.



DFG Forschergruppe 1346

Dynamical Mean-Field Approach
with Predictive Power for
Strongly Correlated Materials

Autumn School
Hands-on LDA+DMFT
4 – 7 October 2011
Forschungszentrum Jülich

DFG Deutsche Forschungsgemeinschaft

JÜLICH FORSCHUNGSZENTRUM

German Research School for Simulation Sciences

Soon after the discovery of quantum mechanics, it became evident that the fundamental obstacle to explaining the properties of solids from *first-principles* is the description of electronic many-body effects. A crucial step forward was density-functional theory (DFT) and its local-density approximation (LDA).

The success of DFT in explaining the physical and chemical properties of solids is so remarkable, that DFT is considered the "standard model" of solid-state physics. Nevertheless, LDA and its generalizations fail for systems in which electrons loose their individuality and whose low-energy properties are dominated by electron-electron correlations: Mott-insulating transition-metal oxides, Kondo and heavy-fermion materials, organic crystals, and many others. The realistic description of such strongly-correlated systems remains, to date, one of the grand-challenges of condensed matter-physics.

During the last years a major breakthrough came with the development of the LDA+DMFT method. In this approach, conventional ab-initio schemes based on DFT/LDA are combined with a modern many-body approach, the dynamical mean-field theory (DMFT).

The present school aims at introducing students starting from the advanced graduate level to this state-of-the-art approach.

Lectures

Overview and Introduction

- Electron correlations and DMFT
- Model Hamiltonians
- Density-functional theory and basis functions
- Experimental challenges

The LDA+DMFT Approach

- Wannier functions and hopping integrals
- The screened U: cLDA and cRPA
- Dynamical Mean-Field Theory
- LDA+DMFT

DMFT Quantum-Impurity Solvers

- Hirsch-Fye Quantum Monte Carlo
- Continuous-time QMC
- Exact diagonalization and Lanczos

Beyond LDA+DMFT

- Cluster DMFT and dual Fermions
- GW+DMFT

Hands-on Sessions

- Wannier functions and model Hamiltonians
- Dynamical Mean-Field Theory
- Hirsch-Fye and continuous-time QMC
- Screened Coulomb parameters

General Information

Venue: The school will take place in the Lecture Hall of the Peter Grünberg Institute at the Forschungszentrum Jülich from 4 to 7 October 2011.

Participation: The school is intended for advanced graduate and PhD students in the field of electronic structure of materials.

Admission: Interested students should apply before May 15, 2011 via internet at the address www2.fz-juelich.de/iff/correl11. Accepted applicants will be informed via e-mail shortly after the deadline for applications.

Accommodation: Applicants can apply for financial support to cover accommodation costs. Participants supported by the school will be accommodated in the Aachen Youth Hostel www.aachen.jugendherberge.de. Funding for accommodations is limited to about 30 students. Preference will be given to students from nodes of the DFG Research Unit 1346.

Computers: Computers for the tutorials will be available for a limited number of participants. Students are encouraged to bring their own laptops.

Transport: A shuttle bus will be operating in the mornings and evenings between the Hostel in Aachen and the Forschungszentrum Jülich.

Hotels in Aachen and Jülich: Participants for whom no low-cost accommodation can be found or who wish to stay in a hotel may find hotels in Jülich or Aachen through the web-sites www.aachen-tourist.de and www.juelich.de/hotelsundpensionen.