

Hands-on-Course KKR band structure and spectroscopy calculations

ORGANIZERS:

Hubert Ebert, Diemo Ködderitzsch (Munich) and Walter Temmerman (Daresbury)

ABSTRACT

The workshop aims at introducing theoreticians as well as experimentalists to the use of the KKR bandstructure method and its applicability to the calculation of spectroscopic properties of magnetic solids. A number of lectures will be given to provide the formal background. During the afternoon sessions the participants will have the opportunity to familiarise themselves with the Munich SPR-KKR program package and its user interface XBAND.

SCIENTIFIC SUMMARY

The multiple scattering formalism formulated in the KKR band structure method is the standard basis for the calculation of spectroscopic properties of solids. Its fully relativistic version allows dealing with linear and circular magnetic dichroism in magnetic solids. The Munich SPR-KKR package provides a corresponding implementation that allows its user to investigate a wide range of systems (compounds, alloys, films or clusters) as well as a large number of ground state and spectroscopic (x-ray absorption, photoemission, x-ray scattering etc.) properties. As it is fully automatised and supported by a graphical user interface it is well suited to be used by experimentalists to complement their investigations by corresponding calculations.

As a matter of fact, our previous hands-on courses were always overbooked and the number of users of the SPR-KKR package increases continuously.

With the forthcoming workshop we want to publish our next public release of the SPR-KKR package that will contain several new features. The most important ones are the full-potential mode for arbitrary lattices, the LDA+U method and the LSDA+DMFT method. The latter feature will be interesting for investigations of correlated systems. For that purpose an efficient DMFT-solver based on the FLEX-scheme will be provided which, in particular, allows performing self consistent calculations.

MEETING PROGRAM

10th – 12th October 2007

University of Munich, Dept. of Chemistry and Biochemistry

The program will consist of talks during the morning sessions. These will review the KKR multiple scattering formalism, its application to the calculation of spectroscopic properties as well as recent developments in electron spectroscopy. The afternoons will be used for practical exercises introducing the participants to the use of the graphical user interface XBAND and the Munich SPR-KKR package.

PRELIMINARY LIST OF LECTURERS (to be confirmed)

P. H. Dederichs, Jülich
H. Ebert, München
O. Sipr, Prague
M. Lüders, Daresbury
D. Szotek, Daresbury
W. M. Temmerman, Daresbury
R. Zeller, Jülich

We expect about 30 participants and about 14 lecturers:

Curriculum Vitae

Prof. Dr. Hubert Ebert

University of Munich

- 28th Sept. 1955 born in Ellwangen/Jagst (Germany)
- 1st Oct. 1976 start of studying Physics at the Ludwig-Maximilians-Universität in München
- March 1982 Diploma in Physics at the Ludwig-Maximilians-Universität in München
- since 1983 research visits (among others) with:
Dr. H. Winter, Kernforschungszentrum Karlsruhe (Germany)
Prof. Dr. P. Weinberger, TU Wien (Austria)
Prof. Dr. P.-H. Dederichs, KFA Jülich (Germany)
Dr. W. Temmerman, Daresbury Laboratory (Great Britain)
Dr. F. Herman, IBM San Jose (USA)
Prof. B. Johansson, Univ. Uppsala (Schweden)
Prof. D. D. Johnson, Urbana (USA)
- 11th Oct. 1983 married with Luise Ostertag
- 1st March - 31st July 1984 research visit with Prof. P. Weinberger at the Technische Universität in Wien (Austria)
- 22nd Feb. 1986 Ph.D. at the Institut für Physikalische Chemie of the Ludwig-Maximilians-Universität in München
- 1st Oct. 1986 - 31st July Post-doc with Prof. B. L. Gyorffy at the University of Bristol (Great Britain)
- 1st Aug. 1987 - 31st March 1993 employed at the Central Research Laboratories of Siemens AG, Erlangen (Germany)
- 12nd Nov. 1990 Habilitation at the Institut für Physikalische Chemie of the Ludwig-Maximilians-Universität in München

since 1st April 1993

Professor for Theoretical Physical Chemistry at the Institut für Physikalische Chemie of the Ludwig-Maximilians-Universität in München

Mai 1996

research visit with Prof. H. Akai as a fellow of the *Japan Society for the Promotion of Science* at the Department of Physics of the University of Osaka (Japan)

Recent publications

1. H. Ebert und Mankovskyy
Field-Induced Magnetic Circular X-Ray Dichroism in Paramagnetic Solids:
A New Magneto-Optical Effect
Phys. Rev. Letters **90**, 077404 (2003).
2. Z. Major, S. B. Dugdale, R. J. Watts, G. Santi, M. A. Alam, S. M. Hayden,
J. A. Duffy, J. W. Taylor, T. Jarlborg, E. Bruno, D. Benea und H. Ebert
Direct observation of the multisheet Fermi surface in the strongly correlated
transition metal compound ZrZn₂
Phys. Rev. Letters **92**, 107003 (2004).
3. J. Minar, H. Ebert, C. de Nadai, N. B. Brookes, F. Venturini, G. Ghiringhelli,
L. Chioncel, A. I. Lichtenstein und M. I. Katsnelson
Observation and theoretical description of the pure Fano-effect in the valence-
band photoemission of ferromagnets
Phys. Rev. Letters **95**, 166401 (2005).
4. M. Kosuth, V. Popescu, H. Ebert und G. Bayreuther
Magnetic anisotropy of thin Fe films on GaAs
Europhys. Lett. **72**, 816 (2005).
5. S. Polesya, O. Sipr, S. Bornemann und J. Minar and H. Ebert
Magnetic properties of free Fe clusters at finite temperatures from first
principles
Europhys. Lett. **74**, 74 (2006).