Research Networking Programmes

Science Meeting – Scientific Report

***Proposal Title*:** **Workshop on the full-potential linear muffin-tin orbital method and dynamical mean-field theory for correlation effects in solids**

***Application Reference N°*:** **4604**

1 Summary

A workshop on density functional theory (DFT) and dynamical mean-field theory (DMFT) as implemented in the full-potential linear muffin-tin orbital (FP-LMTO) code RSPt. The workshop had a strong emphasis on tutorials and hands-on sessions at the computer to familiarize participants with the computational methods, particularly emphasizing problems concerning magnetism, heavy elements and strong-correlation physics within the LDA+DMFT framework. LDA+DMFT has been applied with great success to a wide set of problems particularly to compounds containing magnetic transition metals, lanthanides and actinides, where often both correlation and relativistic effects need to be addressed. The workshop aimed to bring these more advanced methods to a larger circle of DFT practitioners not in immediate contact with groups where development takes place. The participants also had the opportunity to present their own work in oral presentations.
Tutorials, intended for PhD students and researchers interested in learning to handle these techniques, were held each afternoon. Participants in the tutorial sessions were also encouraged to bring own research problems suitable for the course, to get guidance in setting them up with RSPt. Additional problems were provided for further in-depth study and a course certificate provided for students who completed these.

Description of the scientific content and discussions

The workshop programme was planned to progress from straightforward density functional theory (DFT) calculations in standard approximations to increasingly complex questions concerning electron correlation and the uses of dynamical mean-field theory (DMFT). The theoretical progression in the presentations roughly matched the contents of the tutorial sessions held in the afternoons on Tuesday to Thursday.
The programme started on Monday evening with talks on general methodological issues in DFT by A.E. Mattsson (Sandia), J. M. Wills (Los Alamos), V. Havu (Aalto), M. Kuisma (Tampere) and T. Björkman (Aalto) interspersed with a talk on rare-earths clusters by L. Peters (Nijmegen).
The Tuesday programme featured applications of, and challenges for plain DFT calculations from A. Delin (KTH) and M. Ijäs (Aalto) followed by presentations on electron-magnon coupling and transition metal oxides by A. Marmodoro (MPI-Halle) and S. Majumdar (Aalto). The afternoon tutorial session gave an introduction on how to run basic calculations with the RSPt code package.
The Wednesday started with a talk by M. Heikkinen (Aalto) giving a general introduction to DMFT, followed by talks on the implementation of the LDA+DMFT method by O. Grånäs (Uppsala), I. di Marco (Uppsala) and A. Östlin (KTH). This was followed by the second tutorial session, which introduced more advanced concepts like structural relaxation and LDA+U calculations.
On Thursday, further more advanced topics were covered, including talks on the exact diagonalization technique by A. Harju (Aalto) and P. Thunström (Uppsala) and a talk on how to find appropriate interaction parameters from DFT calculations by O. Janson (National Institute of Chemical Physics and Biophysics, Estonia). The tutorial session covered the running of LDA+DMFT in the less time-consuming SPTF approximation, which allows for production scale runs in the limited timeframe of a single tutorial session.
The Friday program was centred on developers' discussions of the future of the RSPt code, led by O. Eriksson (Uppsala).

2 Assessment of the results and impact of the event

This small workshop had a modest set of goals, which it managed to achieve. This is most straightforwardly assessed directly in terms of the four main aims stated in the original ESF/Psi-K application. In addition to these, a secondary beneficial effect was the very positive interaction between members of the strong computational materials science groups at Uppsala University (O. Eriksson) and the Aalto University (the COMP centre of excellence, R. Nieminen), opening up for further future collaborations.

1) A primary aim for the workshop is to bring the LDA+DMFT to a larger circle of DFT practitioners not in immediate contact with groups where development of these methods takes place.

This goal was achieved, with a strong local participation from Finnish universities. The workshop reached the intended audience and gave the opportunity for participants to

discuss how to attack their own research problems using LDA+DMFT as implemented in RSPt.

2) The workshop will have a strong emphasis on tutorials and hands-on sessions at the computer to familiarize participants with the computational methods, particularly emphasizing problems concerning magnetism, heavy elements and strong-correlation physics within the LDA+DMFT framework.

The tutorial sessions held at the CSC IT Centre for Science were largely successful. The participants learned the basics of running the RSPt code in standard DFT mode as well as employing LDA+DMFT. The participants were for most part satisfied with the tutorials.

3) The participants will also get the opportunity to present their own work. Participants in the tutorial sessions will also be encouraged to bring own research problems suitable for the course to get guidance with setting them up with RSPt. Additional problems will be provided for further in-depth study and a course certificate will be provided for students who complete these.

Most participants gave oral presentations of their own work, providing an inspirational orientation for the participating developers in the background of people with a need and an interest in the application of the LDA+DMFT methodology. The tutorial participants came with varying previous experience, but had for most part clear ideas of their intended application of the methods. As almost all participants were above the doctoral student level, only one course certificate was requested.

4) One session will be devoted to developers' discussions concerning future development of the code.

A discussion session with all developers of the RSPt code was held on the last day of the workshop, led by Olle Eriksson. It was concluded that the most important task for the future is to improve the user friendliness of the RSPt code package and to consolidate the advances achieved so far, rather than implementation of new theory. Informal discussions between developers in smaller groups, an important aspect, were also held throughout the workshop.

3 Appendices

Programme of the meeting

Monday 26
-12.00 Arrival and registration
12.00 Lunch
13.30 Opening of the workshop
14.00 A. E. Mattsson, Sandia National Laboratories: *Improving the predictive power of density functional theory calculations*
14.45 J. M. Wills, Los Alamos National Laboratory: *Accurate calculation of materials properties using RSPt/RSPt-Dirac*
15.00 Coffee
15.30 V. Havu, Aalto University: *FHI-aims: an all-electron full-potential electronic structure package*
16.15 L. Peters, Radboud University Nijmegen: *Rare-Earth clusters: How many 4f-electrons do they have?*
16.45 M. Kuisma, Tampere University of Technology: *Model potential approximations for semiconductor band gaps: case GLLB-SC*
17.15-17.45 T. Björkman, Aalto University: *Handling your crystal structure data with CIF2Cell – Laziness has never been easier!*
19.00 Dinner

Tuesday 27
9.00 A. Delin, Kungliga Tekniska Högskolan: *Graphene NEMS*
9.45 M. Ijäs, Aalto University: *Challenges for the theoretical description of graphene-metal systems*
10.15 Coffee
10.45 A. Marmodoro, Max Planck Institute of Microstructure Physics: *From electrons to magnons to electrons: towards a first-principles description of magnon-electron coupling effects*
11.15 S. Majumdar, Aalto University: *Complex oxide materials and their application in spintronics*
11.45 Lunch
13.30-17.30 Tutorials (CSC)

Wednesday 28
9.00 M. Heikkinen, Aalto University: *Real-space DMFT study of finite temperature stability and dimensional crossover of exotic superfluidity in optical lattices*
9.45 O. Grånäs, Uppsala University: *Conserving and non-conserving approximations to solving the impurity problem: Impact on orbital magnetism and total energy properties*.
10.15 Coffee
10.45 I. di Marco, Uppsala University: *Recent development and future challenges in DMFT within RSPt*
11.15 A. Östlin, Kungliga Tekniska Högskolan: *Development of the EMTO+DMFT method*
11.45 Lunch

13.30-17.30 Tutorials (CSC)
19.00 Dinner+Sauna

Thursday 29
9.00 A. Harju, Aalto University: *Introduction to exact diagonalization*
9.45 C. Etz, Uppsala University: *Assessment for strength of electron correlations in SrRuO3*
10.15 Coffee
10.45 P. Thunström, Techniche Universität Wien: *Multi-orbital 2-particle Green's function from the exact diagonalization impurity solver: Preliminary results*
11.15 O. Janson, National Institute of Chemical Physics and Biophysics, Estonia: *Evaluation of microscopic model parameters for magnetic insulators: a computational approach*
12.00 Lunch
13.30-17.30 Tutorials (CSC)
19.00 Dinner

Friday 30
9.00 O. Eriksson, Uppsala University: *Some thoughts on RSPt and electronic structure theory*
9.30 Developers discussions
10.15 Coffee
10.45 Developers discussions + Tutorial cleanup
12.00 Closing of the workshop + Lunch

Full list of speakers and participants

Convenors

Torbjörn Björkman, Aalto University
Olle Eriksson, Uppsala University

Speakers

Oscar Grånäs, Uppsala University
Igor di Marco, Uppsala University
Anna Delin, Kungliga Tekniska Högskolan
Ari Harju, Aalto University
Ville Havu, Aalto University
Miikka Heikkinen, Aalto University
Mari Ijäs, Aalto University
Ann E. Mattsson, Sandia National Laboratories
John Wills, Los Alamos National Laboratory
Lars Peters, Radboud University Nijmegen
Patrik Thunström, Technische Universität Wien
Mikael Kuisma, Tampere University of Technology

Participants

Weijia Fan, Aalto University
Sayani Majumdar, Aalto University
Tuomas Rossi, Aalto University
Divya Srivastava, Aalto University
Tuomas Vanhala, Aalto University
Oleg Janson, National Institute of Chemical Physics and Biophysics, Estonia
Kari Ruotsalainen, University of Helsinki
Andreas Östlin, Kungliga Tekniska Högskolan
Alberto Marmodoro, MPI-Halle