3.1.2 Report on 2008 Tutorial Hands-on-FPLO

IFW Dresden, Germany

24-28 August, 2008

Sponsored by

Psi-k Network
IFW Dresden e. V.
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The 2008 Tutorial Hands-on-FPLO was the seventh tutorial of its kind, in annual succession. After the 2007 La Plata (Argentina) tutorial, it was again placed at IFW Dresden (2002, 2003, 2004, and 2006 - IFW Dresden, 2005 - UC Davis, California). This time, we combined the tutorial with a workshop called "DFT meets experiment". This way the interaction of computation and experiment on actual topics was demonstrated to young participants. A particular focus was on invited talks given by experimentalists who reported successful collaborations with DFT groups and gave an overview over some of the available techniques that can be combined with electronic structure calculations. In particular, experimental reports were given on quantum oscillations (J. Wosnitza), spectroscopy of organic complexes (M. Knupfer) and rare earth compounds (C. Laubschat), and high-pressure experiments (U. Schwarz).

The theoretical part combined recent research on new functionals for highly correlated magnetic systems (W. Pickett, P. Novák), with further development of electronic structure codes (B. Delley - DMol3, P. Gianozzi - Quantum Espresso, V. Blum - FHI-aims) and specific applications (I. Opahle - magnetic shape memory alloys, A. Mykhaylushkin - Fe-alloys under earth's core conditions, A. Tsirlin - low dimensional spin systems, F. Tasnádi - piezoelectricity, M. Gruner - magnetic clusters, H. Eschrig - superconducting Fe-pnictides, D. Kasinathan and H. Rosner - orbital order, B. Hamad - magnetic multi-layers). Eleven contributed talks and several posters completed the program. Most of the lectures can be downloaded from http://www.fplo.de/workshop/ws2008/index.html.

The total number of participants, 59, was higher than in the previous meetings. The tutorial was attended by 27 of the participants, which is at the limit of our local possibilities. The setup of the input and specific features of the FPLO code were presented in introductory lessons. Then, the participants were invited to try FPLO-8 (a pre-release) and to perform a number of calculations like convergence tests for numerical settings, modification and re-compilation of the source code, fixed-spin moment calculations, LSDA+U and LSDA+OPC calculations on cuprate oxides and on the magnetic anisotropy of hcp Co, respectively, determination of Heisenberg model parameters, and the magnetic ground state of transition metal dimers. The related tasks and solutions can be downloaded (http://www.fplo.de/workshop/ws2008/index.html). Partly, they repeat recently published FPLO results.

Finally, I would like to thank, on behalf of all organizers, all participants for their contributions

and the funding institutions (Psi-k network and IFW Dresden) for financial support.

Manuel Richter.

Sunday, August 24

19:00 Registration and get-together reception

Monday, August 25

Morning session: Workshop DFT meets Experiment, invited talks

9:00 Helmut Eschrig (Dresden): Opening

9:05 Warren Pickett (Davis): LDA, DMFT, FPLO: The Story of U

9:50 Jochen Wosnitza (Rossendorf): Magnetic quantum oscillations in strongly correlated metals - experimental data meets theoretical predictions

10:35 Coffee

10:50 Pavel Novák (Prague): Spin and orbital polarization in DFT methods

11:35 Ingo Opahle (Frankfurt): Origin of the tetragonal distortion in FePd shape memory alloys

12:20 Lunch break

Afternoon session: Tutorial Hands-on-FPLO (Getting started and installation)

14:00 Getting started with FPLO-8 (Manuel Richter)

15:00 Task I: Convergence of k summation

15:30 Coffee

16:00 Installation and modification of the code (Ulrike Nitzsche)

16:30 Task II: Code modification and installation

17:00 Ressources and performance (N.N.)

17:15 Break

Evening session: Workshop DFT meets Experiment, contributed talks

17:30 Martin Diviš (Prague): Crystal Field calculated for alloys

17:50 Iryna Kondakova (Kiev): Structure optimization with FPLO7: Perovskites and doped II-VI semiconductors

18:10 Erik Ylvisaker (Davis): Charge self-consistency in LDA+DMFT: Application to Yb valence transition

18:30 Sanjubala Sahoo (Duisburg-Essen): Magnetic anisotropy in transition metal clusters

18:50 End of session

Tuesday, August 26

Morning session: Workshop DFT meets Experiment, invited talks

- 9:00 Bernard Delley (Villigen): DMol3 applications from molecules to surfaces and solids
- 9:45 Martin Knupfer (Dresden): Orbital and spin ground state of transition metal phthalocyanines
- 10:30 Coffee
- 10:45 Paolo Giannozzi (Udine): Theoretical design of phthalocyanine-inorganic semiconductor systems for new hybrid materials
- 11:30 Ulrich Schwarz (Dresden): Clash of cultures? Under pressure, experiment meets theory
- 12:15 Lunch break

Afternoon session: Tutorial Hands-on-FPLO (Concept and spin magnetism)

- 14:00 FPLO-8, an all-purpose DFT code (Klaus Koepernik)
- 15:00 Fixed spin moment method (Michael Kuz'min)
- 15:45 Task III: FSM calculation
- 16:00 Coffee
- 16:30 Task III: FSM calculation, continued
- 17:30 Break

Evening session: Workshop DFT meets Experiment, contributed talks

- 17:45 Ismaila Dabo (Marne-la-Vallée): First-principles simulation of electrochemical systems at fixed applied voltage
- 18:05 Ruijuan Xiao (Dresden): Density functional investigation of the dielectric constant for bilayer graphene.
- 18:25 Kemal Özdoğan (Gebze): A comparative study of ferromagnetism in quinternary Heusler alloys: Super cell, virtual crystal approximation and coherent potential approximation
- 18:45 End of session

Wednesday, August 27

Morning session: Workshop DFT meets Experiment, invited talks

- 9:00 Arkady Mikhaylushkin (Linköping): Structural properties of $Fe_{1-x}Ni_x$ compressed and heated to the Earth's core conditions
- 9:45 Alexander Tsirlin (Moscow): Unraveling magnetic interactions in low-dimensional spin-1/2 systems
- 10:30 Coffee
- 10:45 Ferenc Tasnádi (Linköping): Piezoelectric tensor of $B_{0.125}Al_{0.875}N$ in the special quasirandom structure model
- 11:30 Markus Gruner (Duisburg-Essen): Large scale ab initio calculations of functional magnetic materials
- 12:15 Lunch break

Afternoon session: Tutorial Hands-on-FPLO (Relativity and correlations)

- 14:00 Four component code (Manuel Richter)
- 14:45 Task IV: Evaluation of orbital moments and magnetic anisotropy
- 15:30 Coffee
- 16:00 LSDA+U method (Klaus Koepernik)
- 16:45 Task V: LSDA+U calculation
- 18:00 Break

Evening session: Workshop DFT meets Experiment, contributed talks

- 18:15 Katrin Koch (Dresden): Electronic structure of AFe_2As_2 and RFeAsO- a comparative study
- 18:35 Miriam Schmitt (Dresden): A joined experimental and theoretical study of the J_1-J_2 Heisenberg square lattice model compounds A_2CuTO_6 (A = Sr, Ba; T = Te, W)
- 18:55 End of session
- 19:30 Workshop Dinner

Thursday, August 28

Morning session: Workshop DFT meets Experiment, invited and contributed talks

- 9:00 Clemens Laubschat (Dresden): Dispersing 4f-states: LDA meets Anderson
- 9:45 Volker Blum (Berlin): Tackling biomolecular (secondary) structure with numeric atom-centered orbitals in the FHI-aims code framework
- 10:30 Coffee
- 10:45 Helmut Eschrig (Dresden): Electronic structure of superconducting iron-pnictides
- 11:30 Deepa Kasinathan (Dresden): Orbital order in low-dimensional spin 1/2 systems
- 11:50 Bothina Hamad (Amman): Exchange Coupling and Magnetic Properties of Fe/Ir Multilayers
- 12:10 Lunch break

Afternoon session: Tutorial Hands-on-FPLO (Large systems and molecules)

- 14:00 Approach to complex problems (Helge Rosner)
- 14:10 Evaluation of model parameters (Helge Rosner)
- 14:40 Task VII: Model parameters
- 15:30 Coffee
- 16:00 Task VII: Model parameters (cont.)
- 17:00 Molecules (Manuel Richter)
- 17:10 Task VI: Small molecule
- 17:40 Break

Evening session: Workshop DFT meets Experiment, contributed talks

- 18:00 Małgorzata Samsel-Czekała (Wrocław): Electronic and magnetic structure FPLO studies of U_2N_2 (N = P, As, S, Se) and U_2N_2 (N = Sb, Bi, Te) compounds having the highest Neel and Curie temperatures among uranium systems
- 18:20 Daniel Fritsch (Dresden): Magnetic properties of transition metal dimers
- 18:40 Closing

Friday, August 29

Departure or individual excursions

Posters will be displayed during the whole workshop, poster discussion is intended during the coffee breaks.

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