

0.1 Report on Workshop Magnetism in Complex Systems

Vienna University of Technology, Vienna, Austria

16.-18. April 2009

Ψ_k , **Austrian Ministry of Science and Research, TU-Wien**

Peter Mohn and Jürgen Hafner

<http://www.cms.tuwien.ac.at/>

Our workshop was intended to cover both the theoretical and the experimental aspects of magnetism. To this end we invited speakers and participants from both sides of the gap and finally 50 scientists met in Vienna in order to learn from each other. The experimental side covered basic questions like how to measure magnetic properties (Hilscher) and the thermodynamic aspects of magnetism (Michor). Two lectures gave emphasis to EMCD (Stöger-Pollach, Leifer). Spectroscopic methods were represented by one lecture about the determination of magnetic structures from neutron scattering (Rotter) and one lecture about spin resolved PES (Dedkov). Finally Havela gave an overview about the magnetism of heavy elements, followed by a respective theoretical account by Shick. The theoretical part started with an introduction into magnetism within the LDA (Mohn) and about DMFT and results for various applications (Held). Post DFT methods and the application of hybrid functionals were covered by two lectures by Franchini and Kresse. Szunyogh gave an introduction into relativistic effects and Eriksson reported about ab-initio spin dynamics. Following these more methodological lectures applications were presented which covered Verwey transitions (Blaha), magnetism on grain boundaries (Sob), magnetism from non-magnetic elements (Arita), Magnetic nanostructures on surfaces (Lounis), and in low dimensional systems (Eyert). The field of magnetism in biological systems was covered by a lecture about magnetic ordering in porphyrin molecules (Panchmatia). Turek reported about spin-polarized transport and Kudrnovsky about DMS. The magnetism of small aggregates was discussed for Mn-nanostructures (Zeleny) and transition-metal dimers and ad-atoms (Blonski). Finally Khmelevskyi tried to remove the aura of miracoulocity from the old and ever new Invar problem. All participants were invited to present their own work so that we ended up with 10 posters, which had to be presented as a micro-poster-presentation to the full audience (micro-poster-presentation means that any poster has to be introduced within 3 minutes by showing not more than 2 slides, just enough to raise the interest). The social part of the program included all lunches and coffee breaks as well as the conference dinner. Although Vienna has also a high touristic appeal, the meeting remained very well attended until the very end and was regarded as highly interesting and useful to all participants.

PROGRAMME

Thursday, 16. April 2009

8.30 Registration

9.00-9.05 Hafner: Welcome address

9.05-9.50 Mohn: Magnetism and electronic structure (LDA).

9.50-10.35 Hilscher: Basic aspects of magnetic measurements.

10.35-11.00 Coffee break

11.00-11.45 Michor: Thermodynamic measurements in magnetic systems;
specific heat, dilatometry, and alike

11.45-12.30 Šob: Magnetism on grain boundaries.

12.30-13.30 Lunch

13.30-14.15 Stöger-Pollach: Detection of magnetic properties on the
nanometer scale.

14.15-15.00 Leifer: Probing the electronic nanocosmos in the electron
microscope: Measurements in semiconductor quantum structures and
magnetic materials.

15.00-15.30 Coffee break

15.30-16.15 Blaha: Magnetic and charge order phase transition in
YBaFe₂O₅ (Verwey transition)

16.15-17.00 Dedkov: Spin-resolved photoelectron spectroscopy of magnetic
objects: Principles and recent applications.

Friday, 17. April 2009

9.00-9.45 Held: Dynamical Mean Field Theory (DMFT) and applications.

9.45-10.30 Franchini: Magnetism in metal oxides by post-DFT methods.

10.30-11.00 Coffee break

11.00-11.45 Kresse: Hybrid functionals: Dilute Magnetic Semiconductors.

11.45-12.30 Lounis: Magnetic Nanostructures on Surfaces.

12.30-13.30 Lunch

13.30-14.15 Arita: Theoretical materials design of ferromagnets comprising
non-magnetic elements.

- 14.15-15.00** Szunyogh: Spin-orbit induced phenomena in nanomagnetism.
- 15.00-15.30** Coffee break
- 15.30-16.15** Havela: 5f magnetism and its specific features.
- 16.15-17.00** Shick: Electronic structure and spectral properties of actinides: *f*-electron challenge.
- 17.00-17.45** Panchmatia: Substrate induced magnetic ordering and switching of the metal centre in porphyrin molecules, for application in Spintronics.
- 18.00-19.00** Poster micro presentation followed by postersession.
- 19.15-** Conference Dinner

Saturday, 18.April 2009

- 9.00-9.45** Eriksson: Atomistic spin-dynamics.
- 9.45-10.30** Rotter: Magnetic neutron scattering.
- 10.30-11.00** Coffee break
- 11.00-11.45** Turek: Spin-polarized transport properties of bulk and layered systems.
- 11.45-12.30** Kudrnovsky: Electronic, magnetic, and transport properties of diluted magnetic semiconductors: (Ga,Mn)As as a case study.
- 12.30-13.30** Lunch
- 13.30-14.15** Eyert: Magnetism in low-dimensional systems; From frustration to complex order.
- 14.15-15.00** Zeleny: Noncollinear magnetism in Mn nanostructures.
- 15.00-15.30** Coffee break
- 15.30-16.15** Blonski: Magnetic anisotropy of transition-metal dimers and isolated adatoms on non-magnetic substrates.
- 16.15-17.00** Khmelevskiy: Theory of magnetostriction in Invar materials.

NOTE *Most of the presentations can be downloaded as ppt or pdf from the www-page given above!*

POSTER PRESENTATIONS

Ali Al-Zubi: Complex magnetism of Fe monolayers on hexagonal substrates.

Giovanni Barcaro, Alessandro Fortunelli and Falko Netzer:
Theoretical analysis of the Kondo effect in Cobalt atoms adsorbed on Cu surfaces.

Katarzyna A. Kacprzak, Lauri Lehtovaara, Jaako Akola, Olga Lopez-Acevedo, Hannu Häkkinen: Electronic structure effects of a palladium impurity in a thiolate protected gold cluster.

Alessio Meyer and R. Dovesi: Magnetic interactions in $\text{Ca}_3\text{Y}_2\text{G}_3\text{O}_{12}$ garnets from first principles (Y= Cr, Fe; G= Si, Ge).

Robert Hammerling: High magnetic multipole moments from ab-initio calculations.

Josef Redinger and Peter Mohn: An interface between two non-magnetic metals turns magnetic: The case of YCo_2 (111)/Cu(111).

Lucas Fernández Seivane, Diego Carrascal and Jaime Ferrer:
Magnetism and magnetic anisotropies of small structures containing 5d atoms.

A. Uldry, M. Samaras, R. Iglesias, M. Victoria, W. Hoffelner: From Iron-Chromium to Steel.

Andrei Reyes-Huamantínco, Andrei Ruban, Peter Puschnig, and Claudia Ambrosch-Draxl: Temperature dependence of the stacking fault energy in the Fe-22.5at% Mn alloy: An ab-initio study.

V. Drchal, J. Kudrnovsky, and I. Turek: Electronic, magnetic, and transport properties of semi-Heusler (Cu,Ni)MnSb alloys.

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