Report on

Summer School 'Nanomagnetism and Spintronics'

September 5–13, 2008

Prague, Czech Republic

http://cmd.karlov.mff.cuni.cz/Spintronics-2008/

Scientific organizing committee

I. Turek – Charles University, Prague, and Academy of Sciences of the Czech Republic, Brno J. Kudrnovský – Academy of Sciences of the Czech Republic, Prague P. Bruno – European Synchrotron Radiation Facility, Grenoble

Sponsors

Marie Curie Psi-k Training in Computational Nanoscience ESF – Towards Atomistic Materials Design (Psi-k)





1 Summary

The summer school 'Nanomagnetism and Spintronics' took place from September 5 - 13, 2008 at the Faculty of Mathematics and Physics, Charles University in Prague, Czech Republic.

The scientific part of the school was organized by

- I. Turek (Faculty of Mathematics and Physics, Charles University, Prague),
- J. Kudrnovský (Institute of Physics, Academy of Sciences of the Czech Republic, Prague),P. Bruno (European Synchrotron Radiation Facility, Grenoble, France).

The local organization was carried out by members of the Department of Condensed Matter Physics, Faculty of Mathematics and Physics, Charles University, Prague (I. Turek, Š. Sechovský) and of the Institute of Physics, Academy of Sciences of the Czech Republic, Prague (J. Kudrnovský).

In total, there were 158 participants of the school: 127 students, 28 speakers and 3 scientific organizers.

The purpose of the school was to give an introduction to nanomagnetism and spintronics, with emphasis put on first-principles theoretical methods on the level appropriate to early-stage researchers (last year PhD students, fresh postdocs). The scientific scope included important topics, such as diluted magnetic semiconductors, hybrid systems, spindependent transport properties, effects of finite temperatures, spin dynamics, magnetism of nanostructures, relativistic effects, and electron correlations.

Majority of the participants (both lecturers and students) came from the community of *ab initio* electronic structure theory but a part of the talks was devoted to other theoretical approaches (non-equilibrium Green's functions, model Hamiltonians) as well as to relevant experimental techniques and results (STM, AFM).

2 Description of the scientific content

The school programme, extending over eight days, was based on 28 invited lectures with two inserted poster sessions. The lecturers were allotted sufficient time (90 minutes) to include an introductory part of their topic, physical backgrounds and technical details of the methods used, as well as ample illustrations of application to interesting physical problems. The school lectures were given by 28 outstanding scientists:

Bernard Barbara (Institut Néel, CNRS, Grenoble, France) Gerrit E. W. Bauer (Delft University of Technology, The Netherlands) Silke Biermann (CPHT, École Polytechnique, Palaiseau, France) Gustav Bihlmayer (Forschungszentrum Jülich, Germany) Stefan Blügel (Forschungszentrum Jülich, Germany) Patrick Bruno (European Synchrotron Radiation Facility, Grenoble, France) Carlo Carbone (Istituto di Struttura della Materia, Trieste, Italy)

Hubert Ebert (Ludwig-Maximilian-University, Munich, Germany) Claude Ederer (Trinity College, Dublin, Ireland) Olle Eriksson (Uppsala University, Sweden) Jaroslav Fabian (University of Regensburg, Germany) Albert Fert (Unité Mixte de Physique, CNRS/Thales, Palaiseau, France) Bryan Gallagher (University of Nottingham, UK) Peter Grünberg (Forschungszentrum Jülich, Germany) Pavel Jelínek (Institute of Physics, Acad. Sci. Czech Rep., Prague) Tomáš Jungwirth (Institute of Physics, Acad. Sci. Czech Rep., Prague) Paul J. Kelly (University of Twente, Enschede, The Netherlands) Jan Mašek (Institute of Physics, Acad. Sci. Czech Rep., Prague) Ingrid Mertig (Martin-Luther-University, Halle, Germany) Leonid Sandratskii (MPI for Microstructure Physics, Halle, Germany) Stefano Sanvito (Trinity College, Dublin, Ireland) Jairo Sinova (Texas A&M University, USA) Bedřich Velický (Charles University, Prague, Czech Rep.) Karel Výborný (Institute of Physics, Acad. Sci. Czech Rep., Prague) Peter Weinberger (Center for Computational Nanoscience, Vienna, Austria) Daniel Wortmann (Forschungszentrum Jülich, Germany) Wulf Wulfhekel (University of Karlsruhe, Germany) Jörg Wunderlich (Hitachi Cambridge Laboratory, UK)

The lectures of the school covered a wide area of theoretical magnetism (the whole programme is given in **Appendix I**). The topics addressed by the speakers included:

- spin-dependent transport properties (P. J. Kelly, S. Sanvito, D. Wortmann, G. E. W. Bauer),
- non-collinear magnetic structures (L. Sandratskii, I. Mertig),
- nanoscale magnetic systems (H. Ebert, C. Carbone, P. Bruno, B. Barbara),
- dilute magnetic semiconductors (B. Gallagher, T. Jungwirth, O. Eriksson, J. Mašek),
- effects of spin-orbit interaction on ground-state properties (G. Bihlmayer, P. Weinberger),
- transport phenomena due to spin-orbit interaction (J. Fabian, J. Wunderlich, J. Sinova, K. Výborný),
- advanced experimental techniques and their theoretical background (S. Blügel, P. Jelínek, W. Wulfhekel),
- electron systems far from thermodynamic equilibrium (B. Velický), with strong electron correlations (S. Biermann), and with more than one order parameter (C. Ederer).

Two lectures by Nobel prize winners (A. Fert, P. Grünberg) provided an excellent overview of development of spintronics from the discovery of the giant magnetoresistance effect towards the very recent and possible future applications. All lectures stimulated a number of questions by the students; the following discussions continued mostly during the coffee and lunch breaks.

Electronic files with full contents of the presented lectures were collected and made available to the participants; they can be downloaded at

http://cmd.karlov.mff.cuni.cz/Spintronics-2008/lectures.php
using the password: mellon

In addition to the lectures, two poster sessions were organized so that the young researchers could show results of their own work. More than one half of the students presented a poster; the interesting topics and results displayed led to very lively discussions during both poster sessions (the list of posters is given in **Appendix II**).

3 Conclusion

The school was substantially overscribed and a part of the applications had unfortunately to be rejected (mainly for nationality restrictions imposed by the rules of the Marie Curie Psi-k Training project for the financial support of the students); this large number of students' applications witnesses that the choice of the school topic was really up-to-date. Undoubtedly, the school has motivated a number of young people to enter the field of spintronics and its *ab initio* theoretical description. Moreover, the list of teachers, the pedagogical and scientific level of their lectures, the big number of presented posters, as well as informal contact between students and teachers proved unambiguously that the school was successful.

Photographic impressions



Figure 1: Prof. A. Fert during his lecture.



Figure 2: Prof. P. Grünberg with participants of the summer school.

Appendix I: School Programme

Friday,	September	5

17:00-20:00 registration

Saturday, September 6

9:00 P. H. Dederichs: *Opening*

- 9:00–10:30 P. J. Kelly: Ab initio scattering theory from wave-function matching
- 10:30-11:00 coffee break
- 11:00–12:30 B. Velický: Introduction to non-equilibrium Green's functions

12:30–14:00 lunch

- 14:00–15:30 S. Sanvito: Magnetic tunnel junctions under bias
- $15:30{-}16:00$ coffee break
- 16:00–17:30 D. Wortmann: Complex band structures and all-electron transport calculations for magnetic tunnel junctions

Sunday, September 7

- 9:00–10:30 L. Sandratskii: First-principles study of non-collinear magnetism: Basic principles and applications
- 10:30-11:00 coffee break
- 11:00–12:30 H. Ebert: Finite magnetic metallic clusters
- 12:30-14:00 lunch
- 14:00–15:30 C. Carbone: Nanoscale magnets at surfaces
- 15:30-16:00 coffee break
- 16:00–17:30 I. Mertig: Non-collinear magnetic nanowires

Monday, September 8

- 9:00–10:30 A. Fert: Variations on themes in spintronics: from the roots to recent developments
- 10:30-11:00 coffee break
- 11:00–12:30 G. Bihlmayer: Spin-orbit effects at magnetic surfaces

12:30-14:00 lunch

- 14:00–15:30 P. Weinberger: Magnetic anisotropies in nanostructured matter
- 15:30-16:00 coffee break
- 16:00–17:30 J. Fabian: Interfaces between ferromagnetic metals and semiconductors: spin-orbit coupling and structural symmetry
- $19:00-22:00 \ school \ dinner$

Tuesday, September 9

9:00–10:30 B. Gallagher: Ferromagnetic semiconductors

10:30-11:00 coffee break

11:00–12:30 T. Jungwirth: Ferromagnetic semiconductors for spintronics: Theory concepts and experimental overview

12:30-14:00 lunch

- 14:00–15:30 O. Eriksson: Diluted magnetic semiconductors from a first principles point of view
- 15:30-16:00 coffee break
- 16:00–17:30 J. Mašek: Electronic and atomic structure of dilute magnetic semiconductors (some open questions)

Wednesday, September 10

- 9:00–10:30 P. Bruno: Controlling self-organization and magnetism of nanostructures on surfaces by using quantum interferences
- 10:30-11:00 coffee break
- 11:00–12:30 G. E. W. Bauer: Spin transfer by charge and heat currents
- 12:30-14:00 lunch
- 14:00–16:00 poster session I

Thursday, September 11

- 9:00–10:30 J. Wunderlich: Voltage controlled spintronics effects based on spin-orbit interaction
- 10:30-11:00 coffee break

- 11:00–12:30 J. Sinova: Anomalous Hall transport: merging semiclassical and microscopic theories
- $12{:}30{-}14{:}00 \ lunch$
- 14:00–15:30 K. Výborný: Anisotropic magnetoresistance in diluted magnetic semiconductors
- 16:00–18:00 poster session II

Friday, September 12

- 9:00–10:30 S. Blügel: Spinpolarized scanning tunneling microscopy
- 10:30–11:00 coffee break
- 11:00–12:30 W. Wulfhekel: Spin-polarized scanning tunneling microscopy and spectroscopy: High resolution magnetic imaging and beyond
- $12:30-14:00 \ lunch$
- 14:00–15:30 B. Barbara: Molecular magnets
- 15:30-16:00 coffee break
- 16:00–17:30 S. Biermann: Electronic correlations in solids beyond the LDA

Saturday, September 13

- 9:00–10:30 C. Ederer: Multiferroic materials
- 10:30-11:00 coffee break
- 11:00-12:30 P. Jelínek: AFM: a tool for surface science
- $12:30-14:00 \ lunch$
- 14:00–15:30 P. Grünberg: GMR and some of its applications

Appendix II: List of poster presentations

- A. Al-Zubi: Magnetic order and anisotropy of 3d monolayers on Rh(001)
- C. Ataca: Magnetism of Transition Metal Nanowires
- A. Avdonin: The s,p-d exchange constants in ZnMnTeO alloy
- M. S. Bahramy: Theoretical study on phase stability, magnetism and spin-induced transport in CeMnNi₄ intermetallic compound
- P. Balaz: Current-pulse-induced switching of asymmetric spin valve
- S. Blizak: Density Functional Theory of Collinear Magnetism
- P. Buczek: Non-adiabatic spin dynamics of complex magnetic structures
- K. Carva: Spin-transfer torques in noncollinear spin valves: first principles study
- K.-W. Chen: Electron transport through quantum dots with indirect coupling parameter
- C.-L. Chen: Persistent spin current and local spin density in a tubular 2DEG with Rashba spin-orbit coupling
- G. Cheng: Magnetic-field-induced chains of cobalt nanoparticles
- F. Cinti: Monte Carlo Simulations on Thin Rare Earth Films
- M. Cubukcu: Study of Ferromagnetic Metal/Semiconductor Bilayers
- C. Ertler: Self-sustained magnetoelectric oscillations in magnetic resonant tunneling diodes
- C. Etz: Ab-initio magneto-optical properties of bcc Ni/Ni(100)
- D. Fedorov: First-principles calculations of spin relaxation time in metals
- A. Grünebohm: Ab initio examination of Fe/GaAs(110) interfaces with respect to spin transport
- R. Hammerling: Magnetic multipole moments with $\ell > 1$ in ab-initio calculations
- B. Hardrat: Unique playground for complex magnetism: Fe on hexagonal transitionmetal surfaces
- S. Heers: Lifetime reduction of surface states induced by impurity scattering
- J. Hellsvik: Dynamics of diluted magnetic semiconductors from atomistic spin dynamics simulations
- L. Herrera Diez: Magnetic Anisotropy and Domain Structure in (GaMn)As
- P. Horley: Influence of magnetic field pulses with different time profiles on the magnetization dynamics of a monodomain ferromagnetic particle
- M. Hortamani: Ab initio study of the exchange interactions and Curie temperature of thin film MnSi/Si(001)
- D. Iusan: Theoretical study of Co clustering in ZnO
- M. James: Relativistic embedding and surface electronic structure
- J. Kaczkowski: Ab initio calculations of magnetic properties of wurzite $Al_{1-x}TM_xN$, (TM = V, Cr, Mn, Fe, Co, Ni)
- G. Kaur: Current Induced Dynamic Nuclear Polarization in III-V Semiconductors
- K. Khazen: Anisotropic relaxation of magnetization in GaMnAs thin layers
- L. Kilanski: Room temperature ferromagnetism in $Zn_{1-x}(Mn, Co)_x GeAs_2$ semiconductor: structural, magnetic and transport properties

- R. Klepaczko: The studies of paramagnetic molecules deposited on HOPG (0001) substrates for ESN-STM measurements
- F. Körmann: Importance of magnetism for the thermodynamics of bcc iron: an ab initio study
- P. Krukowski: The studies of organic radical molecules deposited on Au(111) and HOPG (0001) substrates for ESN-STM measurements
- D. Krychowski: Spin-polarized transport through T-shaped DQD system in spinorbital Kondo regime
- J. Kudrnovský: Relation of Curie temperature and conductivity: (Ga,Mn)As alloys as a case study
- D. Legut: Angular dependence of the Xray circular and linear dichroism in transitional metals from first principles
- I. Maznichenko: Electronic and magnetic properties of doped ZnO
- M. Menzel: Electronic properties of bi-atomic Fe chains on Ir(001)
- S. H. Mirhosseini: Electron correlation effects in the magnetoresistance of Fe/MgO/Fe tunnel junctions: First-principles calculations
- C. Neise: Orbital polarization corrections applied to selected uranium compounds
- C. S. Olariu: Investigation of Switching Region in SAF System
- T. Ossowski: Cohesion and magnetism at grain boundaries in chromium
- P. Petkova: Influence of the transition metal impurities on the magnetooptical effect in Bi₄Ge₃O₁₂
- S. Polesya: Temperature Dependence of Magnetic Order in Fe/(Ga,Mn)As Studied by Monte Carlo Simulation
- S. Power: Finite size effects in magnetically doped graphene nanoribbons
- M. Rasander: Structural, chemical and magnetic properties of ternary transition metal carbides
- E. Rozkotová: Ultrafast laser spectroscopy of GaMnAs
- F. Römer: In situ g-factor and magnetic anisotropy determination of Fe/InAs(100)
- H. Sahin: Spin-dependent Conductance of Short Graphene Nanoribbons
- S. Schmaus: Electron transport across single phthalocyanine molecules
- S. Schönecker: fcc bcc epitaxial Bain path of uranium
- T. Schuh: Measuring of magnetic anisotropy of transition metal clusters on Pt(111)
- V. Sessi: Magnetism of surface supported 3d and 4d metal nanostructures
- A. Sidorenko: NMR study of magnetic properties of thin magnetic layer in various interfaces
- B. Spisak, M. Woloszyn: Computer simulation of the spin-polarised transport through a nanodevice
- A. Stroppa: Hybrid functionals applied to Mn doped III-V semiconductors
- V. Stsefanovich: Magnetization process and magnetic anisotropy of (Ga,Mn)As thin films on GaAs (311)A substrate
- A. Thiess: Magnetically suppressed chain formation in break junctions
- S. Trudel: Amorphous iron oxide: Magnetism and structure

- I. Turek: Relativistic electronic structure of (Ga,Mn)As
- E. Wachowicz: Cr segregation at Fe $\Sigma 5(210)$ and $\Sigma 3(111)$ grain boundaries
- A. Werpachowska: Spin waves, anisotropies and Curie temperature in ferromagnetic (Ga, Mn)As
- M. Werwinski: Ab initio studies of antiferromagnetism in UPdAs₂
- A. Wysocki: Effect of magnetic short-range order and local moment softening on spin-disorder resistivity
- P. X. Xu: Influence of Roughness and Disorder on Spin Transfer Torque in Magnetic Tunneling Junctions
- A. Zacarias: DFT approach to molecular electronics
- M. Zelený: Ab initio study of structural and magnetic properties of manganese nanowires from one to three dimensions
- H. Zhang: Surface magnetic anisotropy in external electric fields: Density functional calculations