

Report on Workshop Computational Magnetism and Spintronics

Max-Planck-Institute for the Physics of Complex Systems

Dresden, Germany

November 03-07, 2008

Sponsors

MPI-PKS, psi-k.org, and ESF

Organizers

Olle Eriksson – University of Uppsala, Sweden,

Ingrid Mertig and Peter Zahn – Martin-Luther-Universität Halle, Germany

<http://www.mpi-pks-dresden.mpg.de/~ccms08>

Summary

The workshop was organized at the Max-Planck-Institute for the physics of complex systems in Dresden. Financial support of the Max-Planck-Institute, the psi-k.org network and the ESF Activity 'Towards Atomistic Materials Design' is kindly acknowledged. The workshop was attended by about 90 scientist from 22 countries from Europe and overseas. They presented new theoretical developments and methods, and actual experimental results in 30 talks. Nearly all participants took the chance to present their own results on 52 posters. This provided an inspiring atmosphere for discussions and lively exchange of ideas, which were centered at computer simulations of known, as well as brand new spintronics phenomena. This includes the understanding of the magnetic order and dynamics of nanostructures, spin dynamics under the influence of magnetic and electrical fields, the currently discovered Spin Hall effect, and the behavior of electrons in graphene.

Scientific content, discussions

The addressed topics of the invited talks were:

- Spin Hall Effect (Stern, Buhmann, Jin, Bruno)
- Graphene (Katsnelson, Józsa, Louie, Nieminen, Kelly)
- Multiferroics (Picozzi, Alexe, Ederer, Garcia, Ravindran, Dörr)
- Electronic correlation effects (Schulthess, Temmermann, Lichtenstein)
- Magnetic structures and spin dynamics (Blügel, Wulfhekel, Nordström)
- Diluted magnetic semiconductor (Sanyal, Sato)

- Spin dependent transport (Turek, Ebert, Györffy, Heiliger, Resta, Tosatti)

In addition, a full list of talk titles is given below in the programme section.

Concerning spin Hall and anomalous Hall effect, highly sophisticated experiments were presented to discriminate intrinsic and extrinsic sources of the effect. For the theoretical description of the phenomena a combination of semiclassical transport theory with a quantum theoretical description of the electronic states was proposed as a promising way. This includes the consideration of quantum mechanical model systems as well as parameter-free ab initio calculations. The concept of Berry phases was widely discussed in connection with spin and electron dynamics but also to describe static material properties from first principles. In the graphene section the influence of the degeneracy of the material band structure and the possible magnetism of defects and adatoms were discussed. The considerations of multiferroica were aimed on the control of an electron spin by an electric current or voltage by means of the magnetoelectric coupling provided by the intrinsic material properties or a combination of different of materials. Further investigations exploit the 4 remanent states of a ferromagnetic and ferroelectric tunnel barrier for a 2-bit logic device. The importance of Dzyaloshinski-Moriya interaction for the formation of complex magnetic structures in systems with reduced symmetry was discussed. Advanced methods to describe electronic correlations were presented to calculate the phase diagrams of bulk ferromagnets, cuprates and magnetic impurities. Inelastic tunneling spectroscopy investigations gave insight to the spin torque provided by a polarized current. Spin dependent transport in planar junctions and atomic point contacts were considered with special emphasis on the influence of spin-lattice interaction and the magnetic properties. Methods to describe the magnetic order in dilute magnetic semiconductors and the spinodal decomposition were discussed.

Concluding Remarks

In total the conference was very successful. A lot of very interesting and exciting new results were presented. If we restrict ourselves to just two topics, we might mention here in particular the observation of the inelastic tunneling in STM by Wulf Wulfhekel and the calculations for the Kondo effect of adatoms on surfaces by Sascha Lichtenstein. These two examples are also typical for the good mixture between theoretical and experimental presentations at the workshop which is particular important for the progress in the field.

The workshop is the second in a planned series of CompMag meetings, which was started in 2006 in Jülich. The next one will be organized by Stefan Blügel in spring 2010, again in or close to Jülich. We hope that these meetings will become a tradition in Computational Magnetism.

Programme

Monday, November 3

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| 09:00 - 09:20 | Opening by Roderich Moessner and the Organizers |
| 09:20 - 10:00 | Nathaniel Stern
<i>Imaging electrical spin generation and the spin Hall effect in semiconductors</i> |
| 10:00 - 10:40 | Hartmut Buhmann
<i>Spin Hall effects in HgTe quantum well structures</i> |
| 11:10 - 11:50 | Xiaofeng Jin |

Anomalous Hall effect in ultrathin Fe films

- 11:50 - 12:30 Jairo Sinova
Anomalous Hall transport in spin-orbit coupled systems: Merging Keldysh, Kubo and Boltzmann approaches
- 14:00 - 14:40 Balazs L. Gyorffy
Spin-currents and charge-currents induced torques in relativistic quantum mechanics
- 14:40 - 15:20 Ilja Turek
Ballistic torques in non-collinear spin valves
- 15:20 - 16:00 Patrick Bruno
Hall effects, generalized Einstein relation, and Berry phase
- 16:30 - 17:30 CCMS08-Colloquium
Qian Niu
Berry phase effects on spin and charge transport

Tuesday, November 4

- 09:00 - 09:40 Hubert Ebert
A first-principle description of the TAMR in semiconductor/ferromagnet heterostructures
- 09:40 - 10:20 Christian Heiliger
Bias dependence of spin transfer torque in MgO based tunnel junctions: Ab initio calculations
- 11:00 - 11:40 Csaba Józsa
Spin injection and transport phenomena in graphene
- 11:40 - 12:20 Mikhail Katsnelson
Defects in graphene: Electronic structure, magnetism, scattering mechanisms
- 14:00 - 15:30 Poster session I
- 16:00 - 16:40 Steven G. Louie
Computational study of the electronic, magnetic, transport and optical properties of carbon nanostructures
- 16:40 - 17:20 Risto Nieminen
Defect-associated magnetism in nanostructured carbon
- 17:20 - 18:00 Paul Kelly
Graphene and graphite as perfect spin filters
- 18:00 - 18:40 Raffaele Resta
Orbital magnetization in solid state physics

Wednesday, November 5

- 09:00 - 09:40 Walter Temmerman
Disordered Local Moment Picture of Strongly Correlated 3d and 4f systems
- 09:40 - 10:20 Thomas Schulthess
Intricacies of electronic structure calculations in cuprates and other strongly correlated electron systems
- 11:00 - 11:40 Marin Alexe

- Controlling ferromagnetism with an electric field*
- 11:40 - 12:20 Silvia Picozzi
Multiferroic manganites
- 14:00 - 15:30 Poster session II
- 16:00 - 16:40 Claude Ederer
Toroidal moments and magneto-electric coupling: The case of BiFeO_3 versus FeTiO_3
- 16:40 - 17:20 Vincent Garcia
Intrinsic and artificial multiferroic tunnel junctions for spintronics
- 17:20 - 18:00 Ponniah Ravindran
Giant magnetoelectric effect from density functional calculations

Thursday, November 6

- 09:00 - 09:40 Wulf Wulfhekel
Inelastic tunneling spectroscopy as a tool to study magnetic excitations
- 09:40 - 10:20 Stefan Blügel
Homochiral magnetic structures at surfaces
- 11:00 - 11:40 Lars Nordström
Spin dynamics; from a fine to coarse spatial resolution
- 11:40 - 12:20 Erio Tosatti
Magnetic phenomena, spin orbit effects, and electron transport in nanowire contacts, particularly in Platinum
- 14:00 Leaving for the guided city tour and the visit of Panometer Dresden
(<http://www.panometer.de>)

Friday, November 7

- 09:00 - 09:40 Alexander Lichtenstein
Electronic structure and magnetism of correlated materials
- 09:40 - 10:20 Biplab Sanyal
First principles theory of diluted magnetic semiconductors
- 11:00 - 11:40 Kazunori Sato
Control of spinodal decomposition in dilute magnetic semiconductors and computational materials design for semiconductor spintronics
- 11:40 - 12:20 Kathrin Dörr
Reversible strain experiments on strongly correlated oxide films
- 12:20 - 12:30 Closing

List of speakers

Marin Alexe	Halle, DE
Stefan Blügel	Jülich, DE
Patrick Bruno	Grenoble, FR
Hartmut Buhmann	Würzburg, DE
Kathrin Dörr	Dresden, DE
Claude Ederer	Dublin, IR

Vincent Garcia	Paris, FR
Balazs L. Gyorffy	Bristol, GB
Christian Heiliger	Giessen, DE
Xiaofeng Jin	Shanghai, CN
Csaba Józsa	Groningen, NL
Mikhail Katsnelson	Nijmegen, NL
Paul Kelly	Twente, NL
Alexander Lichtenstein	Hamburg, DE
Steven G. Louie	Santa Barbara
Risto Nieminen	Helsinki, FI
Lars Nordström	Uppsala, SE
Silvia Picozzi	L'Aquila, IT
Ponniah Ravindran	Oslo, NO
Raffaele Resta	Trieste, IT
Biplab Sanyal	Uppsala, SE
Kazunori Sato	Osaka, JP
Thomas Schulthess	Zurich, CH
Jairo Sinova	College Station, US
Nathaniel Stern	Santa Barbara, US
Walter Temmerman	Daresbury, GB
Erio Tosatti	Trieste, IT
Ilja Turek	Prague, CZ
Wulf Wulfhekel	Karlsruhe, DE

List of participants

Donat Jozsef Adams	Marin Alexe	Emmanuel Arras
Pio Baettig	Swarnali Bandopadhyay	Cyrille Barreteau
Lars Bergqvist	Orkidia Bilani-Zeneli	Stefan Blügel
Patrick Bruno	Hartmut Buhmann	Karel Carva
Stanislav Chadov	Sudip Chakraborty	Francesco Cricchio
Peter H. Dederichs	S. Dolia	Kathrin Dörr
Manuel dos Santos Dias	Vaclav Drchal	Engin Durgun
Hubert Ebert	Claude Ederer	Olle Eriksson
Dmitry Fedorov	Jonas Fransson	Daniel Fritsch
Vincent Garcia	Martin Gmitra	Martin Gradhand
Oscar Grånäs	Balazs L. Gyorffy	Christian Heiliger
Martina Hentschel	Tilina Herath	Mighfar Imam
Daungruthai Jarukanont	Xiaofeng Jin	Csaba Jozsa
Muthukumar Kaliappan	Hiroshi Katayama-Yoshida	Mikhail Katsnelson
Paul Kelly	Sergii Khmelvskyi	Angela Klautau
Roman Kovacic	Mukul Laad	Alexander Lichtenstein
Steven G. Louie	Samir Lounis	Frantisek Máca

Alberto Marmorodo
Alessio Meyer
Risto Nieminen
Silvia Picozzi
Martin Rohrmüller
Lakshmi Sankaran
Ersoy Sasioglu
Haldun Sevincli
Nirpendra Singh
Nathaniel Stern
Laszlo Szunyogh
Grigory Tkachov
Yoshitaka Uratani
Peter Zahn

Igor Maznichenko
Seyed H. Mirhosseini
Qian Niu
Ponniah Ravindran
Andrea Salguero
Biplab Sanyal
Kazunori Sato
Mahavir Sharma
Jairo Sinova
Rudolf Sykora
Walter Temmerman
Erio Tosatti
Wulf Wulfhekel

Ingrid Mertig
Cesar A. M. Martinez
Natalia Ostrovskaya
Raffaele Resta
Leonid Sandratskii
Saeed Sarkarati
Thomas C. Schulthess
Dinesh Kumar Shukla
Ivetta Slipukhina
Zdzislawa Szotek
Jan Thöne
Ilja Turek
Oleg Yazyev