

COMPUTATIONAL QUANTUM MAGNETISM

PROGRAM

SP/CE



Photo: Design: SuperPhoto Studio, MA.

INVITED SPEAKERS:

W. Antropov (Ames)
K. Belashchenko (Nebraska)
S. Biermann (Palaiseau)
S. Blügel (Jülich)
A. Chubukov (Minnesota)
M. Coey (Dublin)
R. Coldea (Oxford)
O. Eriksson (Uppsala)

C. Felser (Dresden)
A. Georges (Paris)
M. Gingras (Waterloo)
E. Gross (Halle)
G. Jackeli (Stuttgart)
T. Jungwirth (Prague)
M. Katsnelson (Nijmegen)
G. Khaliullin (Stuttgart)

D. Khomskii (Cologne)
C. Lacroix (Grenoble)
F. Mila (Lausanne)
Y. Motome (Tokyo)
L. Nordstrom (Uppsala)
N. Perkins (Minnesota)
W. Pickett (Davis)
M. van Schilfhaarde (London)

S. Sharma (Halle)
I. Solov'yev (Tsukuba)
S. Streltsov (Ekaterinburg)
R. Thomale (Würzburg)
M. Whangbo (N. Carolina)
A. Yaresko (Stuttgart)

The Spice Phenomena Interdisciplinary Center aims to bring together scientists from diverse disciplines and of varying seniority in the broad area of spin related research. Its goal is to break down scientific barriers and foster emergent areas of research that combine the strengths of different fields.

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Computational Quantum Magnetism
22-26 May 2015



Location: Sparkassenakademie Schloß Waldthausen,
Im Wald 1, 55257 Budenheim, Germany
Tel: +49 (0) 6131-145-199 and +49 (0) 6131-145-225

Contact:

Elena Hilp – spice@uni-mainz.de
Phone (office): +49 6131 39 23648
Phone (mobile): +49 171 62 06497

Program

Friday 22 May

AFTERNOON SESSION

13:30-13:50 *Jairo Sinova: Introduction to meeting – open questions, opportunities, SPICE*

14:00-15:00 *Daniel Khomskii (lecture): Orbitals – 2015. Basics and new development*

15:10-15:30 *Coffee Break*

15:30-16:00 *Sergey Streltsov (talk): Orbital-selective behavior in dimerized systems*

16:10-16:40 *Mikhail Katsnelson (talk): Theory of carbon-based magnetism*

16:50-17:10 *Coffee Break*

17:10-17:40 *Mike Whangbo (talk): On the spin orientation*

Break for discussions, etc.

19:00-20:00 *Dinner at Schloß Waldthausen*

20:00-24:00 *Continuing discussions in the common areas.*

Saturday 23 May

MORNING SESSION

9:00-10:00 *Tomas Jungwirth (lecture): Spin-dependent phenomena and device concepts explored in (Ga,Mn)As*

10:00-10:20 *Coffee Break*

10:20-10:50 *Andrey Chubukov (talk): New quantum phases in anisotropic triangular antiferromagnets*

11:00-11:30 *Natalia Perkins (talk): New phenomena due to Kitaev interactions*

11:40-11:50 *Coffee Break*

11:50-12:20 *Giniyat Khaliullin (talk): Magnetism and doping effects in spin-orbit coupled Mott insulators.*

12:30-13:30 *Lunch at Schloß Waldthausen Restaurant*

AFTERNOON SESSION

13:50-15:10 *Posters*

15:20-15:50 **George Jackeli (talk):** *Spin-orbit induced magnetic order and dynamics in insulating iridates*

16:00-16:30 **Alexander Yaresko (talk):** *Anisotropy of exchange interactions in Ir oxides from band structure calculations*

16:40-17:00 *Coffee Break*

17:00-17:30 **Yukitoshi Motome (talk):** *Quantum Monte Carlo study of Kitaev spin liquids*

17:40-18:10 **Radu Coldea (talk):** *Unconventional magnetic order stabilized by Kitaev interactions in the three-dimensional honeycomb polytypes of Li_2IrO_3*

Break for discussions, etc.

19:00-20:00 *Dinner at Schloß Waldthausen (buffet)*

20:00-24:00 *Continuing discussions in the common areas.*

Sunday 24 May

MORNING SESSION

9:40-10:10 **Michel Gingras (talk):** *Has compelling experimental evidence for order-by-disorder at last been found in a frustrated magnetic material?*

10:20-10:40 *Coffee Break*

10:40-11:40 **Alexander Lichtenstein (lecture):** *Magnetism of correlated materials*

11:40-11:50 *Coffee Break*

11:50-12:20 **Ronny Thomale (talk):** *Pseudofermion functional renormalization group*

12:30-13:30 *Lunch at Schloß Waldthausen Restaurant*

AFTERNOON SESSION

14:00-14:30 **Igor Solovyev (talk):** *Origin and microscopic mechanisms of magnetoelectric coupling in multiferroic manganites*

14:40-15:10 **Antoine Georges (talk):** *Hund's metals*

15:20-15:40 *Coffee Break*

15:40-16:10 **Silke Biermann (talk):** *From LDA++ to X+DMFT: strategies for interfacing electronic structure and many-body theory*

16:20-16:50 **Eberhard Gross (talk):** *Ultrafast laser-induced demagnetization of ferromagnetic materials: identifying the mechanism with real-time TDDFT*

Break for discussions, etc.

19:00-20:00 *Dinner at Schloß Waldthausen (buffet)*

20:00-24:00 *Continuing discussions in the common areas.*

Monday 25 May

MORNING SESSION

9:00-10:00 **Radu Coldea (lecture):** *Neutron scattering as a tool to study magnetism*

10:00-10:20 *Coffee Break*

10:20-10:50 **Michael Coey (talk):** *Some puzzles in oxide magnetism*

11:00-11:30 **Frederic Mila (talk):** *Tensor-network algorithms and frustrated quantum magnetism*

11:40-11:50 *Coffee Break*

11:50-12:20 **Lars Nordström (talk):** *Magnetic order in systems with large spin orbit coupling.*

12:30-13:30 *Lunch at Schloß Waldthausen Restaurant*

AFTERNOON SESSION

13:50-15:10 *Posters*

15:20-15:50 **Olle Eriksson (talk):** *Electronic structure and spin-dynamics*

16:00-16:30 **Harald Jeschke (talk):** *Strongly correlated Dirac electrons in electron doped herbertsmithite*

16:40-17:00 *Coffee Break*

17:00-17:30 **Mark van Schilfgaarde (talk):** *Fe and Ni in the quasiparticle self-consistent GW approximation*

Break for discussions, etc.

19:00-20:00 *Dinner at Schloß Waldthausen (buffet)*

20:00-24:00 *Continuing discussions in the common areas.*

Tuesday 26 May

MORNING SESSION

9:00-09:30 *Vladimir Antropov (talk): Quantum spin fluctuations in magnets*

09:40-10:10 *Kirill Belashchenko (talk): Effects of thermal spin fluctuations on the electronic properties of itinerant magnets: Surprises from ab initio calculations*

10:20-10:40 *Coffee Break*

10:40-11:10 *Yuriy Mokrousov (talk): Computational topological spintronics: from Hall effects to chiral skyrmions*

11:20-11:50 *Claudia Felser (talk): Magnetism in Mn-rich Heusler compounds*

12:00-12:30 *Final remarks*

12:30-13:30 *Lunch at Schloß Waldthausen Restaurant*

Poster titles:

Coupling ferroelectricity with spin-valley physics in oxide-based heterostructures,
Paolo Barone

Giant bulk Rashba effect within GeTe and its sensitivity to epitaxial strain : a first-principles study,
Emilie Bruyer

Addressing strong correlations in molecular spintronics,
Andrea Droghetti

Magnetic properties of orthorhombic perovskite manganites,
Natalya Fedorova

Room Temperature Spin Orbit Torques in Ferromagnetic Half-Heusler Materials,
Jacob Gayles

Ferromagnetism in Cu-doped polar and nonpolar GaN surfaces: A DFT study,
Rafael Gonzalez

The polar Kerr effect as a probe of time reversal symmetry breaking,
Martin Gradhand

Periodization in Cluster Dynamical Mean-Field Theory,
Malte Harland

Half Passivated Graphene: an exotic 2D magnetic material,
Shayan Hemmatiyani

Magnetism of FeRh(001) thin films,

Soon Cheol Hong

Kagome odyssey: traversing a treacherous phase diagram,

Yasir Iqbal

Strongly correlated Dirac electrons in electron doped herbertsmithite,

Harald Jeschke

Magnetic interactions in half-metallic chromium dioxide (CrO₂): relative roles of static and dynamic correlations,

Ilya Kashin

Quantum Monte-Carlo study of quantum magnets with single-ion cubic anisotropy,

Yasuyuki Kato

Antiferromagnetic Heusler Alloys: effects of chemical disorder and magnetic frustration,

Sergii Khmelevskiy

Non-local spin correlations in strongly interacting electron systems,

Friedrich Krien

Weyl Spin Liquids,

Kevin O'Brien

Spin Relaxation in Graphene,

Frank Ortmann

Real-time TDDFT calculation of propagator of fermionic Hubbard lattice in comparison with the pole structures of Greens function,

Noejung Park

Propagation of the spin-orbit exciton due to the Jahn-Teller effect in systems with strong on-site spin-orbit coupling,

Ekaterina Plotnikova

Nature of transport gap and magnetic order in zircon and scheelite type DyCrO₄ from first principles,

Avijeet Ray

Longitudinal spin-fluctuations in paramagnetic FeMnCr and FeMnSiAl random alloys,

Andrei Reyes Huamantincó

The role of La displacement in Titanium d_{xy} ferromagnetism at the LaAlO₃/SrTiO₃ double-exchange like mediation,

Sung-Hyon "Sonny" Rhim

Dzyaloshinskii-Moriya interaction in the pyrochlore Lu₂V₂O₇,

Kira Riedl

Structure and Magnetic Order in Multiferroic YBaFeCuO₅,
Andrea Scaramucci

Spin-orbital frustration in molybdenum pyrochlores,
Hiroshi Shinaoka

Transport in Noncollinear Antiferromagnet Ir_xMn_{1-x},
Libor Smejkal

Indirect coupling in graphene nanostructures from exact diagonalization of Hubbard model,
Karol Szalowski

The bulk monopolization in diagonal magnetoelectrics,
Florian Thöle

Anisotropic Magnetic Hamiltonians in High Symmetry Multiorbital Systems from Hund's Coupling,
Steve Winter

Spin-orbit torque in Antiferromagnets,
Jakub Zelezny