

Program



29. Workshop

on

Novel materials and superconductivity

BSFZ Obertraun

9. - 15. Feb. 2014

Sponsored by TU Wien

Location:	Bundessportheim und Freizeitzentrum BSFZ Obertraun Winkl 49 (Oberösterreich) A-4813 Obertraun Tel.: [+43] (6131) 239-0 international Fax: [+43] (6131) 239-423 international
Date:	Arrival: Sunday, February 9, 2014 Departure: Saturday, February 15, 2014

Chairman: **Univ.Prof. Karlheinz Schwarz**
Institut für Materialchemie, Technische Universität Wien
A-1060 Vienna, Getreidemarkt 9/165-TC, Austria
Telephone:+43-1-58801-Ext. 165301 Fax:+43-1-58801-165982
E-mail:kschwarz@theochem.tuwien.ac.at

Programme committee:

B.Batlogg	S.Bühler-Paschen	U.Diebold
P.Knoll	F.Kubel	W.Lang
G.Rupprechter	K.Schwarz	P.Weinberger

World Wide Web: www.wien2k.at/theochem/obertraun/

Scientific Program

Monday, Feb.10, 2014 (Chair: Karlheinz Schwarz)

14:00	Karlheinz Schwarz (TU Wien): <i>Opening, 29th workshop</i>
14:10	Silke Paschen (TU Wien): <i>Thermopower enhancement by encapsulating cerium in clathrate cages</i>
15:10	Coffee Break
15:40	Martin Sterrer (FHI Berlin, Germany): <i>Towards realistic surface science models of heterogeneous catalysts</i>
16:40	Break
16:50	Günther Rupprechter (TU Wien): <i>Surface science models for anode catalysts of solid oxide fuel cells</i>
18:30	Dinner <i>Evening session (chair: Peter Weinberger)</i>
19:30	Markus Wallerberger , P.Gunacker, G.Rohringer, N.Parragh, A.Galler, K.Held (TU Wien): <i>Vertices and local moments in quantum Monte Carlo for general interactions</i>
20:10	Markus Valtiner , B.Shrestha, T.Baimpos (MPI f. Eisenforschung, Düsseldorf, Germany): <i>Force probe experiments to elucidate structure and dynamics at electrified hydrated interfaces</i>

Tuesday, Feb.11, 2014 (Chair: Ewelina Hankiewicz)

14:00 Andrei **Pimenov** (TU Wien):
Magneto optics in topological insulators

15:00 **Coffee Break**

15:30 Grigory **Tkachov** (Univ. Würzburg, Germany):
*Unconventional superconductivity in topological insulators:
In search for Majorana fermions*

16:30 **Break**

16:45 Adrian **Girschik**, F.Libisch, S.Rotter (Univ. Würzburg, Germany):
Topological insulators in the presence of spatially correlated disorder

18:30 **Dinner**

Evening session (chair: Peter Knoll)

19:30 Alexey **Shuvaev** (Univ. Würzburg, Germany):
Electrically tunable Faraday effect in topological insulators

20:10 Klaus **Höll** (Fa. Hoffmann, Bad Goisern, Austria):
Properties and applications of pressure infiltrated aluminium graphite composites

Wednesday, Feb.12, 2014 (Chair: Bertram Batlogg)

14:00 Ewelina **Hankiewicz** (Univ. Würzburg, Germany):
The spin helical transport in topological insulators

15:00 **Coffee Break**

15:30 Dirk **van der Marel** (Univ. Geneve, Switzerland):
Detailed electronic structure of SrTiO₃ : Theory and experiment

16:30 **Break**

16:45 Yasmine **Sassa** (ETH Zürich, Switzerland):
Soft X-ray ARPES of three-dimensional systems

18:30 **Dinner**

Evening session (chair: Peter Blaha)

19:30 **Micro Poster Presentation:** *Each poster can be briefly presented in 3 minutes
PowerPoint presentations need to be arranged with the organizer.*

20:00 **POSTER SESSION**

Thursday, Feb.13, 2014 (Chair: Frank Kubel)

14:00	Klaudia Hradil (TU Wien): <i>Beyond Bragg reflections – crystallographic information from the analysis of disordered scattering</i>
15:00	Coffee Break
15:30	Roland Miletich (Univ. Wien): <i>Novel materials at high pressures? Experimental approach</i>
16:30	Break
16:45	Andrey Zheludev (ETH Zürich, Switzerland): <i>In search of the magnetic Bose glass</i>
18:30	Dinner <i>Evening session (chair: Dirk van der Marel)</i>
19:30	Zhicheng Zhong , Liang Si, K.Held (TU Wien): <i>Switchable giant Rashba effect in complex oxide heterostructures</i>
20:10	Helge Rosner (MPI Dresden, Germany): <i>Interplay of crystal structure and magnetism – how relevant is local magnetism?</i>

Friday, Feb.14, 2014 (Chair: Helge Rosner)

14:00 Rudi **Hackl** (WMI, Garching, Germany):
Phase transitions in iron based compounds

15:00 **Coffee Break**

15:30 Xavier **Rocquefelte**, P.Blaha, K.Schwarz, S.Kumar, J.van den Brink
(IMN Nantes, France):
High pressure cupric oxide: a room temperature multiferroic

16:30 **Break**

16:45 Stefan **Lebernegg**, A.A.Tsirlin, O.Janson, H.Rosner (MPI Dresden, Germany):
Quantum physics meets natural beauty – a study of magnetic Cu(2+)-minerals

18:30 **Dinner**

Evening session (chair: Karlheinz Schwarz)

19:30 Peter **Weinberger**, Ch.Knoll, D.Müller, W.Artner, M.Reissner (TU Wien):
Impact of electronic and steric factors on iron(II) spin cross-over behavior

Posters

- D.Rettenwander, Ch.Geiger, R.Wagner, M.Maier, Georg **Amthauer** (Univ. Salzburg)
The role of dopant cations in $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$: From crystal chemistry to conductivity
- Elias **Assmann** (TU Wien)
What's new with Wannier functions? Recent developments with wien2wannier and woptic
- Andreas **Baum**, T.Böhm, F.Kretzschmar, B.Muschler, J.-H. Chu, I.R.Fisher, R.Hackl (Walther-Meissner-Institut, Garching)
Magnetic and structural phase transition in BaFe_2As_2 studied via Raman spectroscopy
- Bernhard **Bichler** (TU Wien)
Liability of iron (II) PNP pincer complexes k_3 vs k_2 bonding modes of PNP ligands
- Johannes **Bintinger**, E.Horkel, J.Kymissis (TU Wien)
Scope and limitation of palladium catalyzed C-H activation reactions towards novel planarized triphenylamines as organic electronic materials
- Thomas **Böhm**, F.Kretzschmar, R.Hackl, A.F.Kemper, B.Moritz, T.P.Deveraux (Walther-Meissner-Institut, Garching, Germany)
Subdominant d-wave coupling in $\text{Ba}_{0.6}\text{K}_{0.4}\text{Fe}_2\text{As}_2$
- Uladzislau **Dziom** (TU Wien)
How to measure the terahertz Hall-effect in topological insulators
- Christian **Knoll**, D.Müller, G.Giester, J.Ofner, P.Weinberger, G.Steinhauer (TU Wien)
An unusual water-poor 5,5-azobistetrazolate of dysprosium
- J.Weber, H.Krenn, S.Shahzad, K.Ettinger, I,Letofsky-Papst, Peter **Knoll** (Univ.Graz)
Magnetic behavior of NiO-nanoparticles probed with SQUID and Raman spectroscopy
- Eamon **McDermott**, P.Bazylewski, G.S. Chang, L.Van Nguyen, P.Blaha (TU Wien)
Study of spin-polarized behavior in Co-doped grapheme
- Danny **Müller**, Ch.Knoll, M.Reissner, P.Weinberger (TU Wien)
Main group(IV) substituted tetrazoles in Fe(II) spin-cross-over
- Hannes **Puntscher**, D.Lumpi, P.Kautny, B.Stöger, T.Baumgartner, J.Fröhlich (TU Wien / Univ. Calgary, Canada)
Photophysical and electrochemical properties of novel carbazol and indolocarbazol-funczionalized dithienophosphole oxides
- Franz **Renz**, B.Costa, G.Klingelhöfer, B-Sindelar, F.Dencker, B.Dreyer, Y.Tanatsugu (Univ. Hannover, Germany)
The hidden Klimt
- Daniel **Rettenwander**, P.Blaha, R.Laskowski, K.Schwarz, P.Bottke, M.Wilkening, G.Amthauer (Univ. Salzburg)
A DFT study of the role of Al^{3+} in the fast ion conductor $\text{Li}_{7-3x}\text{Al}_{3+x}\text{La}_3\text{Zr}_2\text{O}_{12}$ garnets
- Jacob **Reynvaan**, H.Grünwald, M.Mayer, P.Knoll (Univ.Graz)
Deposition of diamond line carbon with inverted fireballs
- Mohammad **Rezek**, S.Katircioglu (Palestine Techn.Univ.)
Electrical and structural properties of GaN nano wires by density functional theory

Main SPEAKERS

Rudi Hackl

Walther Meissner Institut
Bayrische Akademie d. Wissenschaften
Walter-Meissner-Str. 8
Garching
D-85748, Germany
E-mail: hackl@wmi.badw.de

Ewelina Hankiewicz

Physics Department
Würzburg University
Am Hubland
D-97074 Würzburg
Germany
E-mail: hankiewicz@physik.uni-wuerzburg.de

Klaudia Hradil

X-Ray Center
TU Wien
Getreidemark 9
A-1060 Vienna
E-mail: klaudia.hradil@tuwien.ac.at

Roland Miletich

Institut für Mineralogie und
Kristallographie
Universität Wien
Althanstr. 14
A-1090 Wien
E-mail: roland.miletich-pawliczek@uni-vie.avc.at

Silke Paschen

Institut für Festkörperphysik
TU Wien
Wiedner Hauptstr. 8-10
A-1040 Vienna
E-mail: paschen@ifp.tuwien.ac.at

Andrei Pimenov

Institut für Festkörperphysik
TU Wien
Wiedner Hauptstr. 8-10
A-1040 Vienna
E-mail: pimenov@ifp.tuwien.ac.at

Xavier Rocquefelte

Institute de Matériaux Jean Rouxel
Université de Nantes
Boite Postale 32229
F-44322 Nantes Cedex 3
France
E-mail: xavier.rocquefelte@cnsr-immn.fr

Martin Sterrer

Department of Chemical Physics
Fritz-Haber Institut der MPG
Faradayweg 4-6
D-14195 Berlin
Germany
E-mail: sterrer@fhi-berlin.mpg.de

Grigory Tkachov

Institute for Theoretical and Astrophysics
Würzburg University
Am Hubland
D-97074 Würzburg
Germany
E-mail: Grigory.Tkachov@physik.uni-wuerzburg.de

Dirk van der Marel

Departement de physique de la Matière
Condensée
Université de Genève
Quai Ernest-Ansermet 24
CH 1211 Genève
Switzerland
E-mail: dirk.vandermarel@unige.ch