

Programme



27. Workshop

on

Novel materials and superconductivity

PLANNERALM

11. - 18. Feb. 2012

Sponsored by TU Wien

Location:	Planneralm , Ennstal (Steiermark) A-8953 Donnersbach
	Tel.: [+43] (3683) 3167 or 3168 international
	Fax: [+43] (3683) 31674 or 31684 international
	(03683) 3167 or 3168 within Austria
Date:	Arrival: Saturday, February 11, 2012
	Departure: Saturday, February 18, 2012

Chairman: **Univ.Prof. Karlheinz Schwarz**
Institut für Materialchemie, Technische Universität Wien
A-1060 Vienna, Getreidemarkt 9/165-TC, Austria
Telephone:+43-1-58801-Ext. 15670 Fax:+43-1-58801-15698
E-mail:kschwarz@theochem.tuwien.ac.at

Programme committee:

C.Ambrosch-Draxl B.Batlogg S.Bühler-Paschen
P.Knoll F.Kubel W.Lang
K.Schwarz P.Weinberger

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

Plenary Lectures

Sunday, Feb.12, 2012 (Chair: K. Schwarz)

9:00	K. Schwarz (TU Wien): <i>Opening, 25th workshop</i>
9:10	Günther Rupprechter (TU Wien): <i>Understanding catalytic properties via surface science studies</i>
10:20	Coffee Break
10:40	Philip Moll (ETH Zürich, Switzerland): <i>Mass renormalization in Fe-pnictides and related compounds</i>

Monday, Feb.13, 2012 (Chair: B. Batlogg)

9:00	Joachim Sauer (Humboldt Univ. Berlin, Germany): <i>Atomistic understanding of heterogeneous catalysis: Quantum chemistry in concert with experiment</i>
10:00	Coffee Break
10:30	Alois Loidl (Univ. Augsburg, Germany): <i>Superconductivity and magnetism in iron-selenide compounds</i>

Tuesday, Feb.14, 2012 (Chair: P. Knoll)

9:00	Bertram Batlogg (ETH Zürich, Switzerland): <i>Research Integrity</i>
10:00	Coffee Break
10:30	Ernst Bauer (TU Wien): <i>From superconductivity towards thermoelectricity: Germanium based skutterudites</i>

Wednesday, Feb.15, 2012 (Chair: Claudia Ambrosch-Draxl)

9:00 Ulrike **Diebold** (TU Wien):
*Surface science investigation of metal oxides:
Looking with STM and understanding with DFT*

10:00 **Coffee Break**

10:30 Cristiana **Di Valenti** (Univ. di Milano-Biocca, Italy):
Vis-light activation of semiconducting oxides

Wednesday, Feb.15, 2012 (Chair: W. Lang)

13:00 Jürgen **Fleig** (TU Wien):
*Electrochemical energy conversion:
From fundamentals to future applications*

14:30 **Coffee Break**

15:00 Andrei **Pimenov** (TU Wien):
Metamaterials and negative refraction

Thursday, Feb.16, 2012 (Chair: P.Blaha)

9:00 Alexander **Boris** (MPI Stuttgart, Germany):
*The difference between thin and very thin :
Control of electron flow and magnetism in atomically thin transition metal oxides*

10:00 **Coffee Break**

10:30 Raimund **Podloucky** (Univ. Wien):
*First-principles studies of the thermodynamic stability of solid phases
including lattice vibrations*

Evening sessions

Sunday, Feb.12, 2012 (Chair: R.Hackl)

19:00	Xavier Rocquefelte (CNRS Nantes, France): <i>Modelling of organic-inorganic hybrid materials</i>
19:40	Hermann Kronberger (TU Wien): Mechanistic aspects of surface structuring via electrodeposition

Monday, Feb.13, 2012 (Chair: K. Held)

19:00	Johannes Ferber (Univ. Frankfurth a Main, Germany): <i>Effects of correlation in an LDA+DMFT framework: The iron pnictides LiFeAs and LiFeP</i>
19:30	Markus Aichhorn (TU Graz, Austria): <i>From 3d to 4d to 5d: Surprising behavior of transition metal oxides</i>
20:00	Andrei Pimenov (TU Wien): <i>Terahertz properties of the Fe(SeTe) superconductor</i>

Tuesday, Feb.14, 2012 (Chair: A. Pimenov)

19:00	Philipp Hansmann (École polytechnique, Paris, France): <i>Adatom systems on the silicon 111-surface: Mott or not ?</i>
19:40	Wolfgang Lang (Univ. Wien, Austria): <i>Vortex motion in YBCO with intrinsic and artificial order modulations</i>

Wednesday, Feb15, 2012 (Chair: P. Blaha)

19:00	Micro Poster Presentation: <i>Each poster can be briefly presented in 3 minutes PowerPoint presentations need to be arranged with the organizer.</i>
19:30	POSTER SESSION

Thursday, Feb.16, 2012 (Chair: X. Rocquefelte)

19:00	Karsten Held (TU Wien): <i>LDA+DMFT: From bulk to nanostructures</i>
19:30	Peter Weinberger (TU Wien): <i>Spin transitions above room temperature A synthetic breakthrough in tetrazole ligand synthesis</i>
20:00	Mohammad Rezek (Palestine Techn. Univ): <i>Electronic structure and phase transition in $Sc_xAl_{1-x}N$ alloys</i>

Friday, Feb.17, 2012 (Chair: B. Batlogg)

19:00	Aliaksei Charnukha (MPI Stuttgart, Germany): <i>Optical conductivity of 122 iron pnictides</i>
19:40	Elias Assmann (TU Wien): <i>Correlated heterostructures for fun and profit: Bulk and interface properties of Lanthanum vanadate</i>

Posters

- Tzvetanka **Boiadjieva**, H.Kronberger, T.Szeck, M.Monev, T.Lavric (CEST, Wr.Neustadt)
Novel Zn-Cr alloys: Alloy deposition for corrosion protection in stage of industrial trials
- Hans-Martin **Eiter**, M.Lavagnini, R.Roßner, R.Hackl, E.A.Nowadnick, A.F.Kemper, T.P.Devereaux, J.-H.Chu, J.G.Analytis, I.R.Fisher (WMI, Garching, Germany),
Charge density waves in $ErTe_3$
- Jürgen **Fleig**, T.Tröml, H.Hutter (TU Wien)
Oxygen diffusion in donor-doped Lead Zirconate Titanate (PZZ)
- Jakob **Kanter**, P.Moll, F.Ronning, E.Bauer, B.Batlogg (ETH Zürich, Switzerland)
Electric transport measurements on micro-structured $CePt_2In_7$ single crystals in a diamond anvil cell
- Florian **Kretzschmar**, B.Muschler, T.Böhm, A.Baum, R.Hackl, V.Tsurkan, A.Loidl, J.Deisenhofer, T.P.Devereaux, J.-H.Chu, J.Analytis, I.R.Fisher, MaiHu Wen (Walther-Meissner-Institut, Garching, Germany)
Pairing in FeAs systems
- Christian **Knoll**, D. Müller, P.Weinberger, B.Stöger (TU Wien)
New tetrazole compounds as asymmetric ligands for mixed iron(II) lanthanide complexes
- Stefan **Lebernegg**, M.Schmitt, O.Janson, A.Tsirlin, H.Rosner (MPI CPFS Dresden, Germany)
Magnetism of Cu^{2+} chain-compounds - how covalency matters
- G.Tondi, A.Petutschnigg, M.Demker, Maurizio **Musso** (Univ.Salzburg)
Tannin based organic foams and their characterization by Raman spectroscopy
- Anna **Pimenov**, Ch.Kant, V.Tsurkan, A.Loidl, A.H.Vasiliev, L.Svistov, L.A.Prozorova, A.Pimenov (TU Wien)
Synthesis and magnetic dynamics of multiferroic chromates
- Franz **Renz**, G.Vanko, P.Homenya, R.Sadaat, N.Zoltan, S.Houtari (Univ.Hannover)
Hard x-ray induced thermal hysteresis
- F.Renz, G.Vanko, P.Homenya, R.Sadaat, N.Zoltan, Yakup **Baran** (Univ.Hannover)
Hard x-ray induced excited spin state trapping
- F.Renz, G.Vanko, P.**Homenya**, R.Sadaat, N.Zoltan, S.Houtari (Univ.Hannover)
Strong field hard x-ray induced excited spin state trapping
- Julia **Stelzl**, N.Hassan, P.Weinberger, G.Molnar, A.Bousseksou, F.Kubel, K.Mereiter, R.Boca, W.Linert (TU Wien)
Spectroscopic, structural and magnetic investigations of iron(II) complexes based on 1-isopropyl- and 1-isobutyl-substituted tetrazole ligands
- Julia **Weber**, F.Shahzad, K.Nadeem, H.Krenn, P.Knoll, K.Ettinger, I.Letofsky-Papst (Univ.Graz)
Magnetic properties of NiO nano-particles

Main SPEAKERS

Bertram Batlogg
Solid State Physics Laboratory
ETH Zürich
HPF F9
Hönggerberg
CH-8093 Zürich
Switzerland
E-mail: batlogg@phys.ethz.ch

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

Alexander Boris
Max Planck Institut für
Festkörperforschung
Heisenbergstr. 1
D 70569 Stuttgart , Germany
E-mail: A.Boris@fkf.mpg.de

Ulrike Diebold
Institut für Angewandte Physik
TU Wien
Wiedner Hauptstr. 8
A-1040 Vienna
E-mail: diebold@iap.tuwien.ac.at

Cristiana Di Valenti
Dip. Di Scienza dei Materiali
Università di Milano-Bicocca
via Cozzi 53
I-20125 Milano
Italy
E-mail:
christina.divalentin@mater.unimib.it

Jürgen Fleig
Institute for Chemical Technologies and
Analytics
Vienna University of Technology
Getreidemarkt 9/164EC
A-1060 Vienna
E-mail: j.fleig@tuwien.ac.at

Alois Loidl
Experimental Physics V
Center for Electronic Correlations and
Magnetism
Institute for Materials Resource
Management
University of Augsburg
D-86135 Augsburg, Germany
E-mail:
aloidl@physik.uni-augsburg.de

Philip Moll
Solid State Physics Laboratory
ETH Zürich
HPF F9
Hönggerberg
CH-8093 Zürich, Switzerland
E-mail: phmoll@phys.ethz.ch

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

Raimund Podloucky
Institut für Physikalische Chemie
Universität Wien
A-1090 Vienna, Sensengasse 8/7
E-mail:
raimund.podloucky@univie.ac.at

Günther Ruppachter
Institute for Materials Chemistry
TU Wien
Getreidemarkt 9
A-1060 Vienna
E-mail: grupp@imc.tuwien.ac.at

Joachim Sauer
Institut für Chemie
Humboldt-Universität zu Berlin
Unter den Linden 6
D-1099 Berlin, Germany
E-mail: js@chemie.hu-berlin.de