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# REPORT

Workshop *Electronic properties of spin-orbit driven oxides*, held at the Leibniz Institute for Solid State and Materials Research (IFW) in Dresden from September 4th to September 7th, 2013.

## 1.1 Organizers

### 1. Prof. Dr. Roser Valenti

Responsible for implementation, finances and accounting as required by DFG

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## Summary

In this workshop we brought together scientists in the fields of solid state chemistry, experimental physics, theoretical physics and computational sciences working on the emerging problem of relativistic correlated materials, such as iridates, osmates, etc. These systems present a substantial challenge to theory and experiments since several relevant energy scales converge to the level of 0.5-1 eV: one-electron hopping  $t$ , spin-orbit coupling  $\lambda$ , onsite Coulomb repulsion  $U$ , and Hund's rule magnetic coupling  $J$ . This is often accompanied by nontrivial geometries, such as honeycomb, Kagome, or post-perovskite lattice structures, to mention a few. Many phenomena, intuitively understood in the non-relativistic  $3d$  transition metal oxides or weakly relativistic  $4d$  systems, become nontrivial and challenging in  $5d$  materials. In this workshop the leading researchers from all over the world reported their latest results. And we had ample discussions in the talks and posters.

## Schedule of the workshop and List of Speakers and Participants

The information is attached below.

### 1 Report

The three-day workshop was extremely useful for improving our understanding on  $4d$  and  $5d$  oxide materials. We had overview talks from experimentalists, like the one of P. Gegenwart where we revisited the experimental situation of the family of hexagonal iridates  $\text{Na}_2\text{IrO}_3$ ,  $\text{Li}_2\text{IrO}_3$  and the rhodate  $\text{Li}_2\text{RhO}_3$  (213 compounds). We also had a nice discussion talk from G. Cao on synthesis and the possible phase diagram for  $(\text{Na}_{1-x}\text{Li}_x)_2\text{IrO}_3$ . Y.L. Kim recapitulated in his talk the most important observations through resonant inelastic scattering (RIXS) on iridate-based materials. G. Cao also commented about possible pressure and doping effects on  $\text{Sr}_2\text{IrO}_4$  and the pyrochlore 327 systems. B. Buechner presented a nice review of the electron spin resonance technique (ESR) as applied to  $\text{Sr}_2\text{IrO}_4$ .

We had also many interesting and useful talks on the appropriate modelling for  $4d$  and  $5d$  materials. One of the important topics was the Kitaev model. There was a general consensus that the Kitaev and the Heisenberg-Kitaev models are uniquely interesting in their own right independently whether they are applicable or not to the 213 compounds. These models show a very rich phase diagram that is very sensitive to details. We learnt from N. Perkins that the Kitaev term enhances the so-called zig-zag long range order on the classical J1-J2-J3 Heisenberg phase diagram. S. Rachel and J. Kunes discussed the possible topological and magnetic phases due to the Kitaev term up to second neighbors. L. Hozoi and M. Imada presented a full mapping of the multiband Hubbard model with spin-orbit coupling in the strong-coupling limit to a Heisenberg-

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Kitaev model with anisotropic terms. S. Trebst presented an extension of the Heisenberg-Kitaev model to the triangular lattice and M. Daghofer showed the appearance of phases such as Kitaev-driven vortices. R. Thomale investigated such phase as zig-zag and spiral in the J1-J2-J3 Heisenberg model with a Kitaev term within functional renormalization group theory. H. Jeschke and K. Foyevtsova presented first principles calculations for the 213 systems and discussed the importance of itinerancy in these materials. R. Moessner and P. Horsch concentrated on the magnetic and electronic excitations in the Kitaev and Heisenberg-Kitaev models.

We had many nice talks on first principles studies for the iridate-based materials. S. Biermann and J. Kunes presented LDA+DMFT results. Hae Young Kee discussed the dichotomie of Slater versus Mott insulators and M. Imada, L. Balents, A. Coldea, Yong Baek Kim and A. Subedi concentrated on the importance of frustration effects (pyrochlores, hyper-kagome, double perovskites).

We had also a few very interesting off-topic talks like the one of D. Khomskii on magnetic gold and platinum or D. van der Marel on charge-ordered nickelates. B. Yan presented topological insulators based on Heusler materials and R. Thomale discussed exotic superconductivity in two-dimensional hexagonal systems.

Last but not least, we had beautiful posters with lots of discussion on ab initio optics for iridates (A. Yaresko, Y.Li). On a full magnetic hamiltonian mapping for hexagonal iridates by Y. Yamaji. V. Schnells discussed the 327 systems and L. Savary presented ab initio and model results on the unusual phase diagram of some pyrochlore materials. We had various theoretical approaches by S. Artyukhin, P. Augustinsky, K. Bassis, M. Becker, N. Bogdanov, I. Eremin and V. Katakuri for 4d and 5d materials and we also enjoyed a few experimental posters on RIXS by P. Clancy, ESR by V. Kataev, on synthesis of  $\text{Bi}_2\text{FeCrO}_6$  by A. Khare, on the investigation of band versus topological insulator in  $\text{Sb}_2\text{Se}_3$  by K. Pal and on ARPES experiments on high-Tc superconductors by R. Dhaka.

We believe that the workshop was a success and would like to thank the ESF and PsiK for making the meeting possible.

# Electronic properties of spin-orbit driven oxides

## Organizing Committee

Roser Valenti  
(Frankfurt)

Jeroen van den Brink  
(Dresden)

Igor Mazin  
(Washington)

IFW Dresden

September 4-7, 2013

## Invited speakers:

- L. Balents (Santa Barbara)
  - B. Buechner (Dresden)
  - S. Biermann (Palaiseau)
  - L. Chapon\* (Grenoble)
  - A. Coldea (Oxford)
  - R. Coldea (Oxford)
  - M. Daghofer (Dresden)
  - I. Eremin (Bochum)
  - C. Felser (Dresden)
  - K. Foyevtsova (Oak Ridge)
  - P. Gegenwart (Goettingen)
  - J.P. Hill\* (Brookhaven)
  - L. Hozoi (Dresden)
  - G. Jackeli (Stuttgart)
  - H.O. Jeschke (Frankfurt)
  - G. Khaliulin (Stuttgart)
  - B. J. Kim\* (Argonne)
  - Y. B. Kim (Toronto)
  - Y.-J. Kim (Toronto)
  - D. Khomskii (Cologne)
  - T. Berlijn (Gainesville)
  - J. Kunes (Prague)
  - D. van der Marel\* (Geneva)
  - R. Moessner (Dresden)
  - N. Perkins (Madison)
  - G. Sawatzky (Vancouver)
  - A. Subedi (Palaiseau)
  - H. Takagi\* (Stuttgart)
  - R. Thomale\* (Wurzburg)
  - S. Trebst (Cologne)
- \* To be confirmed



Leibniz-Institut  
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Werkstoffforschung  
Dresden

Deutsche  
Forschungsgemeinschaft

DFG

GOETHE  
UNIVERSITÄT  
FRANKFURT AM MAIN



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Prof. Jeroen van den Brink (local)  
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Dr. Igor Mazin  
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## Workshop

Electronic properties of spin-orbit driven oxides

Dresden, September 4-7, 2013

### Workshop venue:

IFW Dresden  
Helmholtzstraße 20  
01069 Dresden  
Seminar room: D 2E.27



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Leibniz-Institut  
für Festkörper- und  
Materialforschung  
Dresden

## Workshop program

Wednesday, 4<sup>th</sup>

18:00 **Welcome Reception**

IFW Dresden  
Restaurant

Thursday, 5<sup>th</sup>

08:55 **Welcome**

09:00 - 10:30 **Experiment**

Gegenwort

van der Morel

Y.-J. Kim

Honeycomb-lattice Iridates  
Optical properties of strain- and composition tuned  $\text{RNiO}_3$   
Resonant inelastic x-ray scattering investigation of honeycomb Iridates

10:30 - 11:00 **Break**

11:00 - 12:30 **Theory: Materials oriented**

Khomskii

Strong covalency and ligand holes, or how to make magnetic gold?

Imada

Iridates as playgrounds of topological physics

H. Y. Kee

Meta-insulator transition in layered perovskite Iridates: spin-orbit band or Mott Insulators

12:30 - 14:00 **Lunch break**

14:00 - 15:30 **Theory: Model oriented**

Bolens

Theory of novel correlation phenomena in pyrochlore Iridates

Jackeli

Spin-orbit coupling induced novel phases in Mott insulating oxides

Perkins

Finite temperature phase diagram of the classical Kitaev-Heisenberg model

15:30 - 16:00 **Break**

16:00 - 17:30 **Moessner**

Dynamics of a quantum spin liquid -- the dynamical structure factor of Kitaev's honeycomb model

Rachel

Topological and magnetic phases in monolayers of  $\text{Na}_2\text{IrO}_3$

Horsch

Hidden Quasiparticles and Incoherent Photoemission Spectra in  $\text{Na}_2\text{IrO}_3$

17:30 - 19:30 **Poster session**

Snacks & drinks will be served

Friday, 6<sup>th</sup>

09:00 - 10:30 **Experiment**

Gang Cao

Spin-Orbit Coupling Tuned Ground States in Single-Crystal Iridates

Hill

Crystal Fields, Spin-orbit coupling and Electronic Excitations: Resonant Inelastic X-ray Scattering Studies of Iridate Compounds

A. Coldea

Electronic structure of two Iridates as measured by quantum oscillations

10:30 - 11:00 **Break**

11:00 - 12:30 **Theory: Materials oriented**

Kunes

Biermann

Hozoi

Spin-orbit physics of Iridates with  $\text{Wien}2\text{k}$   
A dynamical mean field view on  $\text{Sr}_2\text{IrO}_4$   
Anisotropic magnetic interactions in 4d5 and 5d5 oxides

12:30 - 14:00 **Lunch break**

14:00 - 15:30 **Theory: Model oriented**

Y.B. Kim

RKKY interactions and anomalous Hall effect in metallic pyrochlore Iridates

Trebst

Spin-orbit physics of  $j=1/2$  Mott insulators on the triangular lattice

Thomale

Characterization of spin-orbit driven topological quantum states of matter.

15:30 - 16:00 **Break**

16:00 - 17:00 **Theory: Materials oriented**

Jeschke

Foyevtsova

Daghofer

Electronic structure of honeycomb Iridates and Rhodates  
Competing interactions in  $\text{Na}_2\text{IrO}_3$ : quasi-molecular orbitals, spin-orbit effects, on-site Coulomb correlations  
The spin-orbit coupled  $j=1/2$  antiferromagnet in Iridates

Saturday, 7<sup>th</sup>

09:00 - 10:00 **Experiment**

Büchner

Feiser

Electron spin resonance studies of Iridates  
Heusler compounds, spin orbit coupling, topological insulators and new effects

10:00 - 11:00 **Theory**

Subedi

Electronic structure and magnetism in the post-perovskite  $\text{CaIrO}_3$  and double perovskites  $\text{La}_2\text{ZrIrO}_6$  and  $\text{La}_2\text{MgIrO}_6$

Concluding remarks

## Workshop program

## Poster session

No.	Presented by	Title
1	Artukhin, Sergey	Soliton lattice and Yukawa forces in the rare earth orthoferrite TbFeO <sub>3</sub>
2	Augustinsky, Pavel	Phase Diagram of Two-Band Hubbard Model
3	Bassis, Kenrae Maugem	Effects of colored noise on Landau-Zener transitions: Two- and Three- level systems
4	Becker, Michael	Spin-orbit physics of $J=1/2$ Mott Insulators on the triangular lattice
5	Bogdanov, Nikolay	Interplay of local O-ion distortions and longer-range lattice anisotropy in Sd pyrochlores
6	Clancy, Patrick	Resonant X-ray Studies of Rh-doped Sr <sub>2</sub> IrO <sub>4</sub> : Magnetic Properties of a Doped Spin-Orbital Mott Insulator
7	Dey, Tusharkanti	Effect of high pressure synthesis on the spin-orbit driven Mott insulator Ba <sub>3</sub> Yr <sub>2</sub> O <sub>9</sub>
8	Dhaka, Rajendra Singh	Electronic structure of high temperature superconductors probed by angle-resolved photoemission spectroscopy*
9	Emmanuel, Igunbor	First principle Adsorption and dissociation of hydrogen sulphide from gold cluster.
10	Eremilov, Ilya	Effects of spin-orbit coupling on the itinerant spin response in oxides
11	Kotzev, Vladislav	1) Spin glass magnetism in layered iridates Na <sub>3</sub> -xM <sub>1</sub> Ir <sub>2</sub> O <sub>6</sub> (M = Ni, Zn)
12	Kotzev, Vladislav	2) Antiferromagnetic resonance in the layered iridate Sr <sub>2</sub> IrO <sub>4</sub>
13	Kotukuri, Vamsi	Ab initio quantification of anisotropic magnetic interactions in Ir and Rh oxides
14	Khare, Amit	Growth and properties of Bi <sub>2</sub> FeCrO <sub>6</sub> multiferroic thin film
15	Li, Ying	Analysis of the Microscopic behavior of Na <sub>2</sub> IrO <sub>3</sub>
16	Pal, Koushik	Broken Adiabaticity at a Pressure Induced Electronic Topological Transition from Band to Topological Insulator in Sb <sub>2</sub> Se <sub>3</sub>
17	Sovary, Lucile	Unusual Phase Transition in Conducting Pyrochlore Iridates with All-In-All-Out Magnetic Order
18	Schnells, Vera Irina	Theory of the magnetic properties of the bilayer iridate Sr <sub>3</sub> Ir <sub>2</sub> O <sub>7</sub>
19	Tsirlin, Alexander	Electronic structure of honeycomb-lattice magnet beta-RuCl <sub>3</sub>
20	Yamaji, Youhei	Effective spin models for honeycomb iridium oxides AZrO <sub>3</sub> (A=Na, Li) from ab initio electronic structures
21	Yaresko, Alexander	Optical properties of some iridates from band structure calculations

Notes

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## Participants

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