Chemistry meets Physics in Topology
A workshop for young reserach leaders

Feb1-4, 2017 at Schloss Ringberg

The aim is to bring together international young research leaders from the disciplines of condensed-matter physics and solid-state chemistry.

Organizers:
Binghai Yan (MPI-Dresden)
Leslie Schoop (MPI-Stuttgart)

Invited speakers:

Christian Ast (MPI-FKF Stuttgart)
Mazhar Ali (MPI Halle)
Nurit Avraham (Weizmann)
Andrei Bernevig (Princeton)
Andreas Grüneis (MPI-FKF Stuttgart)
Elena Hassinger (MPI-CPfS Dresden)
Philip Moll (MPI-CPfS Dresden)
Lukas Muechler (Princeton)
Frank Pullman (MPI-PKS Dresden)
Raquel Queiroz (Weizmann)
Andreas Rost (MPI-FKF Stuttgart)
Andreas Schnyder (MPI-FKF Stuttgart)
Leslie Schoop (MPI-FKF Stuttgart)
Tomohiro Takayama (MPI-FKF Stuttgart)
Maia Vergniory (Donostia Inter. Phys. Center)
Binghai Yan (MPI-CPfS, Dresden)
Wolfgang Zeier (University of Giessen)

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Program of Chemistry Meets Physics in Topology, A Workshop for Young Researchers

Max Planck Institute for Solid State Research and Max Planck Institute for Chemical Physics of Solids

Feb 1-4, 2017

Conference site: Schloss Ringberg

Wednesday, Feb-1

12:00	**–**	**23:00**	**Arrival**
18:30			**Dinner**

Thursday, Feb-2 (Talk time: 25 mins presentation + 10 mins questions)

8:00	**–**	**9:00**	**Breakfast**
			Chair: Binghai Yan
09:00	**–**	**09:35**	Philip Moll, MPI-CPfS, Hunting Weyl Fermions in microstructured topological semi-metals
09:35	**–**	**10:10**	B. Andrei Bernevig, Princeton Univeristy, Berry Phases of Berry Phases
10:10	**–**	**10:40**	**Coffee Break**
			Chair: Leslie Schoop
10:40	**–**	**11:15**	Andreas Schnyder, MPI-FKF, Crystalline topological semi-metals
11:15	**–**	**11:50**	Maia Vergniory, Donostia International Physics Center and MPI-FKF, Magnetic non-symmorphic topological insulator realization
11:50	**–**	**14:30**	**Lunch Break and Coffee**
			Chair: B. Andrei Bernevig
14:30	**–**	**15:05**	Christian Ast, MPI-FKF, Dirac Cone Protected by Non-Symmorphic Symmetry and 3D Dirac Line Node in ZrSiS and related compounds
15:05	**–**	**15:40**	Leslie Schoop MPI-FKF, New Dirac and Weyl materials beyond ZrSiS
15:40	**–**	**16:10**	**Coffee Break**
			Chair: Maia Vergniory
16:10	**–**	**16:45**	Raquel Queiroz, Weizmann Institute of Science, Nonsymmorphic semimetals: topological protection of Dirac fermions
16:45	**–**	**17:20**	Lukas Muechler, Princeton, Moebius Molecules, Fragile Mott Insulators and 2D symmetry protected topological phases
17:20	**–**	**17:55**	Andreas Grüneis, MPI-FKF, Ab-initio studies of ZrSiX (X=S,Se,Te) surfaces
18:30			**Dinner**

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Friday, Feb-3

8:00	**–**	**9:00**	**Breakfast**
			Chair: Andreas Rost
09:00	**–**	**09:35**	Ady Stern, Weizmann Institute of Science, Non-local transport in Weyl semi-metals
09:35	**–**	**10:10**	Elena Hassinger, MPI-CPfS, Fermi Surface Topology and Chirality in Weyl Semimetals
10:10	**–**	**10:40**	**Coffee Break**
			Chair: Mazhar Ali
10:40	**–**	**11:15**	Nurit Avraham, Weizmann Institute of Science, Scanning Tunneling Microscopy of Weyl Semimetals
11:15	**–**	**11:50**	Andreas Rost, MPI-FKF, Control and study of 3D Dirac semimetals
11:50	**–**	**14:30**	**Lunch Break and Coffee**
			Chair: Ady Stern
14:30	**–**	**15:05**	Binghai Yan, MPI-CPfS and Weizmann Institute, Dirac nodal lines and induced spin Hall effect in metallic rutile oxides
15:05	**–**	**15:40**	Mazhar Ali, MPI-Halle, A chemist's approach to maximizing the Spin Hall Effect
15:40	**–**	**16:10**	**Coffee Break**
			Chair: Christian Ast
16:10	**–**	**16:45**	Wolfgang Zeier, Giessen University, Thinking like a chemist - Understanding the chemistry behind moving bands in thermoelectrics
16:45	**–**	**17:20**	Benjamin Balke, Stuttgart University, Material design of thermoelectrically highly efficient Heusler compounds using phase separations and nano-composites
18:30			**Dinner**

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Saturday, Feb-4

8:00	**–**	**9:00**	**Breakfast**
			Chair: Andreas Schnyder
09:00	**–**	**09:35**	Frank Pollman, MPI-PKS, Dynamical signatures of quantum spin liquids
09:35	**–**	**10:10**	Tomohiro Takayama, MPI-FKF, Honeycomb iridate as a platform for topological spin liquid
10:10	**–**	**12:00**	**Coffee Break and departure**

Philip Moll (MPI Dresden)

Hunting Weyl Fermions in microstructured topological semi-metals

Topological semi-metals are characterized by crossings of two bands near the Fermi level, leading to a linear dispersion relation in three dimensions. The low energy excitations of the system can be mapped onto the Weyl- and Dirac-Hamiltonian, which provide the quantum mechanical description of relativistic massless Fermions. This unusual band structure is expected to introduce exotic phenomena from relativistic physics into condensed matter experiments, such as the famous axial anomaly and the appearance of quasiparticle chirality as a conserved quantity. Yet this correspondence goes beyond simple duplication of high energy physics, and novel phenomena can appear that are inherently absent in high energy theories: Unlike the free space in the universe, a solid material has a surface. Protected surface states appear at the surface, the “Fermi Arcs”, which provide a pathway connecting Weyl subsystems of opposite chirality. Our group searches for distinct signatures of relativistic quasiparticles in mesoscale crystalline samples of topological materials where the quasiparticle mean free path is comparable to the sample size. These microstructures are fabricated from high quality crystals using Focused Ion Beam machining.

We have observed Shubnikov-de Haas oscillations in microstructures of the Dirac semimetal Cd3As2, whose unusual magnetic field periodicity and finite size effects are in agreement with “Weyl orbits”, the theoretically predicted cyclotron path consisting of Fermi arc and chiral bulk states. While surface state like quantum oscillations are readily observed in samples of rectangular cross-sections, they are absent in triangular samples. This is at odds with oscillations arising from trivial surface states, however can be naturally understood through a length-dependent phase factor leading to destructive interference in samples with non-uniform thickness (triangle). [1]

In addition, we have observed a magnetic anomaly at the quantum limit of topological semimetals that distinctly sets them apart from trivial semi-metals. The key to this bulk topological response is rooted in the zeroth Landau level: A hallmark of topological band-structures is a field independent last Landau level, while that level in a trivial metal retains a field dependence due to zero-point fluctuations. This difference manifests itself as a surprisingly strong magnetic anomaly that we have observed in the Weyl semi-metal NbAs.[2]

[1] P.J.W.M et al., Nature 535, 266-270 (2016); [2] P.J.W.M et al., Nature Communications 7:12492 (2016)

Andrei Bernevig (Princeton University)

Berry Phases of Berry Phases

We extend the celebrated quantum theory of charge polarization - which links the dipole moment in a crystal to the Berry potential of the occupied bands - to classify the long-missing case of quadrupole, octopole and higher moments. We show the symmetries that can provide for quantized multipole moments and present experimental settings in which these can be measured.

Andreas Schnyder (MPI Stuttgart)
Crystalline topological semi-metals

In this talk, I will survey recent developments regarding the topological classification of band-crossings in terms of crystal symmetries. As concrete examples, I will discuss two topological materials: the nodal line-semi metal Ca3P2 and the anti-ferromagnet CuBi2O4. The semi-metal Ca3P2 exhibits a line of Dirac nodes near the Fermi energy. Its topological properties will be examined in terms of a low-energy effective theory, derived from ab-initio DFT calculations. I will discuss the parity anomaly that exists in this nodal-line semimetal and show how it is connected to unusual transport phenomena. The anti-ferromagnet CuBi2O4 exhibits magnetic point-group symmetries as well as non-symmmorphic symmetries. I will show that these symmetries lead to the protection of four-fold degenerate Dirac points and Dirac lines. The monopole charges and the associated surface states of this system will be discussed.

Maia G. Vergniory (MPI Stuttgart; Donostia International Physics Center, ES)
Magnetic non-symmorphic topological insulator realization

Recently, we have realized that spatial symmetries allow for the stabilization of topological phases much more exotic than those that can be found with time-reversal symmetry alone [1]. In this talk I will show that we can find symmetry-protected free fermionic excitations that can occur in condensed matter systems, classified in linear and quadratic 3-, 6- and 8- band crossings stabilized by space group symmetries in crystals with spin-orbit coupling and time-reversal symmetry. However, a material science study and realization of materials did not happen yet. During this talk I will present some realized candidates and a new innovative way of getting the double Fermi arcs at the surfaces of these new non-symmorphic topological materials accompanied by group theory analysis [2].

[1] B. Bradlyn et al. Science 353 (6299), aaf5037
[2] In preparation

Christian Ast (MPI Stuttgart)

Dirac Cone Protected by Non-Symmorphic Symmetry and 3D Dirac Line Node in ZrSiS and related compounds

Materials harboring exotic quasiparticles, such as Dirac and Weyl fermions have garnered much attention from the physics and material science communities. Particularly interesting is a new class of layered materials with a stabilized square lattice and non-symmorphic symmetry, because they can host a new kind of protected Dirac cone, which cannot be gapped by spin-orbit coupling. We show with angle resolved photoemission studies supported by ab initio calculations that the highly stable, non-toxic and earth-abundant material, ZrSiS, has an electronic band structure that hosts several Dirac cones which form a Fermi surface with a diamond-shaped line of Dirac nodes. We also demonstrate that, ZrSiS is not a unique occurrence, but is only a representative of a whole new class of materials exhibiting new types of 2D Dirac cones protected by non-symmorphic symmetry. Interestingly, most of these systems studied thus far feature unforeseen surface states, where some of the non-symmorphic symmetries may be broken. We find that the energy range of the linearly dispersed bands is as high as 2eV above and below the Fermi level; much larger than of any known Dirac material so far. These characteristics make ZrSiS and its sister compounds very promising for future applications.

Leslie Schoop (MPI Stuttgart)
New Dirac and Weyl materials beyond ZrSiS

In this talk I will discuss materials that are structural to the non-symmorphic Dirac line node materials ZrSiS. I will show how chemical strain as well as incorporation of magnetic elements can be used to tune the electronic structure to reach new topological phases.

Raquel Queiroz (Weizmann Institute of Science)
Nonsymmorphic semimetals: topological protection of Dirac fermions

Crystal symmetries have been shown to play a crucial role in the protection of relativistic fermions in lattice models. Their nontrivial topology is evident, among others, by the existence of topological surface states. In this talk I will focus on semimetal systems where nonsymmorphic space group lead to an odd number of Dirac fermions, incompatible with the existence of topologically protected surface states. I will show that a topological invariant is still well defined and fully determined by the crystal symmetry. I will conclude with some remarks on experimental signatures in these systems.

Lukas Muechler (Princeton University)

Moebius Molecules, Fragile Mott Insulators and 2D symmetry protected topological phases

Motivated by the concept of Moebius aromatics in organic chemistry, the Hubbard model on ring-shaped molecules has been shown previously to support a fragile Mott insulator (FMI) ground state. FMIs are insulators cannot be adiabatically connected to a single Slater-determinant state (a band insulator), as long as time-reversal symmetry and point group symmetries are preserved.
In this talk, we discuss two-dimensional lattices of weakly-coupled FMI molecules belonging to multi-dimensional irreducible representations of the molecular point group. The low-energy effective Hamiltonians map onto quantum compass models with broken spin SU(2) symmetry. On the triangular lattice, the ground state develops long-range magnetism, which corresponds to a charge-ordered state of the molecules. On the honeycomb lattice, interestingly, we find a non-degenerate gapped spin-liquid ground state that preserves all spatial symmetries but transforms nontrivially under point-group operations. Our microscopic model therefore realizes an intrinsically interacting fermionic symmetry protected topological (SPT) phase.

Andreas Grüneis (MPI Stuttgart)

Ab-initio studies of ZrSiX (X=S,Se,Te) surfaces

This presentation summarises ab-initio results obtained for the band structure of surfaces of the layered ZrSiX (X=S,Se,Te) compounds. The calculated band structures are compared to experimental findings and the influence of surface adsorbates on surface states is discussed. Furthermore we will discuss the reliability of the employed ab-initio theories and provide an outlook to post-DFT methods.

Ady Stern (Weizmann Institute of Science)

Non-local transport in Weyl semi-metals

In my talk I will discuss several transport phenomena that highlight the non-local aspect of electronic transport in Weyl semi-metals. These include Coulomb drag, interaction with electro-magnetic radiation and non-local voltage-current relations.

Elena Hassinger (MPI Dresden)

Fermi Surface Topology and Chirality in Weyl Semimetals

Weyl Fermions are the solution of the massless Dirac equation [1]. Weyl semimetals are the solid state realization of these massless chiral Fermions. Recently the non-centrosymmetric mono-pnictides (Ta,Nb)(P,As) were predicted to be Weyl semimetals by ab initio DFT calculations [2]. The presence of Weyl nodes and Fermi arc surface states in these materials was later confirmed by ARPES [3]. Here, we present the precise Fermi surface topology of TaP and TaAs as determined by quantum oscillation measurements and ab intio bandstructure calculations. It will be shown that chirality in TaP is ill-defined as the Fermi surface pockets enclose pairs of Weyl points [4]. In TaAs, on the other hand, well-defined Weyl pockets of opposite chirality exist [5]. It is therefore the best candidate known to date where phenomena related to Weyl fermions can be investigated experimentally.

[1] H. Weyl Zeitschrift f. Physik 56, 330 (1929) [2] H. Weng et al. Phys. Rev. X 5, 011029 (2015) [3] B. Q. Lv et al. Phys. Rev. X 5, 031013 (2015), S.-Y. Xu et al. Science 349, 613 (2015) [4] F. Arnold et al. Nat. Comm. 7, 11615 (2016) [5] F. Arnold et al. Phys. Rev. Lett. 117, 146401 (2016)

Nurit Avraham (Weizmann Institute of Science)
Scanning Tunneling Microscopy of Weyl Semimetals

In my talk I will present our recent findings on two topological materials: the Weyl semimetal TaAs and the putative weak and crystalline topological insulator Bi2TeI.
The correspondence between surface “Fermi-arcs” and bulk Weyl cones in a Weyl semimetal uniquely allows to study the notion of bulk surface correspondence. The surface of tantalum arsenide, similar to that of other members of the Weyl semimetal class, hosts non-topological states that obscure the exploration of the Fermi arc states. We use the spatial structure of the surface states’ wave function visualized by scanning tunneling microscopy to distinguish the surface Fermi arcs and to observe their unique properties and their correspondence with the bulk states [1]. While the non-topological states show strong coupling to the lattice structure, we find that the Fermi arcs are only weakly bound to it. We find that the arcs’ energy dispersion shows clear correspondence with the Weyl nodes. We obtain these results using an analysis technique based on the role of the Bloch wave function in shaping quantum electronic interference patterns. At present we are trying to understand new data that we have on the evolution of these interference patterns in magnetic field.
Bi2TeI, is a layered material which was predicted theoretically to be a weak topological insulator (TI) where some of its surfaces are gapped and the others are gapless. Our measurements show one dimensional conducting channels at the steps boundaries, which are consistent with topological surface states on the side surfaces. However on top of the terraces, where the density of states is expected to vanish, we observe non-zero density of states, showing that the surface is in fact gapless. These findings are supported by recent theoretical calculations showing that this surface hosts topological surface states that are protected by Mirror symmetry, making the weak TI also a crystalline TI. We are now trying to nail down the existence of both WTI and TCI phases in this material. The rich structure of quasi 2D terraces and islands obtained on such cleaved Bi2TeI surfaces provides an excellent playground to explore some of the most fundamental concepts of TIs.
[1] http://advances.sciencemag.org/content/2/8/e1600709)

Andreas Rost (MPI Stuttgart)
Control and study of 3D Dirac semimetals

3D Dirac semimetals are promising materials for both applications and the discovery of new phenomena. They have exceptional properties such as ultrahigh mobility and extreme transverse magnetoresistance as well as an apparent large negative longitudinal magnetoresistance. Upon the introduction of a gap these are often topological crystalline insulators hosting topological surface states. The main aim of our research is the control of the physical properties of Dirac semimetals either through chemical substitution or external parameters such as magnetic field. In my talk I will sketch out a broad overview of our advances and plans. In the first part I will discuss our progress on achieving this aim in a family of 3D Dirac electron materials – the inverse perovskites A3BO (A=Ca, Sr, Eu / B=Pb, Sn). Here we can tune (i) the anisotropy of the 3D Dirac dispersion, (ii) the role of spin orbit coupling and (iii) introduce magnetism in the Eu compounds. In the second part of my talk I will introduce our spectroscopic imaging STM studies on the 3D Dirac line node material ZrSiS. In particular I will concentrate how the properties of (i) the bulk Dirac line node and (ii) the unusual surface state originating from symmetry breaking at the surface are reflected in our quasiparticle interference (QPI) signal. For the former we observe unconventional long-range changes to the local density of states whereas for the latter we can track in real space how it is subsiding into the bulk at energies where the surface state and bulk states merge in momentum space. Finally I will give an outlook to how we plan to bring together control over the band structure in magnetic Dirac semi metals with STM studies to directly image the magnetic 'switching' of topological surface states.

Binghai Yan (MPI Dresden)

Dirac nodal lines and induced spin Hall effect in metallic rutile oxides

For metallic rutile oxides IrO_2, OsO_2 and RuO_2, we have found Dirac nodal lines (DNLs) in their band structures and revealed a large spin Hall conductivity contributed by these nodal lines, which explains the strong spin Hall effect of IrO_2 discovered recently [K. Fujiwara et al. Nat. Comm. 4, 2893 (2013)]. Two types of DNLs exist. The first type forms DNL networks that extend in the whole Brillouin zone and appears only in the absence of SOC, which induce surface states on the boundary. Because of the SOC induced band anti-crossing, large intrinsic spin Hall effect can be realised in these compounds. The second type appears at the Brillouin zone edges and is stable against SOC because of the protection of nonsymmorphic symmetry. Besides finding new DNL materials, our work implies that the first type DNLs and the spin Hall effect may be commonly correlated to each other, indicating new guiding principles to search for DNLs in spin Hall effect materials or enhance the spin Hall effect by DNLs in the band structure.

Mazhar Ali (MPI Halle)

A chemist's approach to maximizing the Spin Hall Effect

Spintronic devices have been relatively slow to reach technological adoption partially because of the difficulties in generating spin currents at low power costs. Use of the Spin Hall Effect (SHE) in some materials such as Pt and Beta-W is one of the most promising methods for generating large spin currents. The Spin Hall Angle (SHA; Js/Jc) is a measure of the efficiency of the charge to spin conversion in these materials and it has been calculated that an SHA of > 0.7 (70%) would be sufficient for overcoming the technological roadblock. Increasing the SHA can be approached from the aspect of increasing the strength of the SHE which is intimately tied to the Berry curvature generated by the electronic structure. Here I will outline a chemist's approach to creating thin films of a material with an SHA of > 0.7; maximizing the Berry curvature and correspondingly the SHE through electronic structure engineering via chemical intuition.

Wolfgang Zeier (Giessen University)

Thinking like a chemist - Understanding the chemistry behind moving bands in thermoelectrics

Modifying electronic bands and band engineering has recently become a promising approach in the field of thermoelectrics, however, the underlying reasons are sometimes not well understood. In this seminar we will discuss some of our approaches to understand the underlying structural and bonding reasons for band convergence and band movements in a multitude of semiconducting materials. (1) We will show the structural origin of band convergence in PbTe, due to a stereo-chemical expression of the Pb lone pairs. (2) Further, we will show how crystal symmetry and bonding overlap interactions affect the band degeneracy and band gaps in quaternary chalcopyrites. (3) Finally, we will provide an understanding of how electron doping in $CoSb_3$ leads to changes in the band structure and band convergence, showing that the rigid band approximation does not always hold up in this class of materials.

Benjamin Balke (University of Stuttgart)

Material design of thermoelectrically highly efficient Heusler compounds using phase separations and nano-composites

Half-Heusler compounds are one of the most promising candidates for thermoelectric materials for automotive and industrial waste heat recovery applications. In this talk, I will give an overview about our recent investigations of phase separations in half Heusler thermoelectrics, focusing on the ternary system TiNiSn-ZrNiSn-HfNiSn. I will show how we 8 adapted this knowledge to design a p-type Heusler compound which exhibits a ZT that is increased by 130% compared to the best published bulk p-type Heusler. I will also present how we used the phase separation to design thermoelectric highly efficient nanocomposites of different single-phase materials. Since the price for Hafnium was doubled within the last 15 months, our research focused on the design of half-Heusler compounds without Hafnium. I will present a very recent calculation on ZT per € and efficiency per € for various materials followed by our latest very promising results for n-type Heusler compunds without Hafnium resulting in 20 times higher ZT/€ values. These results strongly underline the importance of phase separations as a powerful tool for designing highly efficient materials for thermoelectric applications that fulfill the industrial demands for a thermoelectric converter. Finally, I will discuss if and how the new topological materials could have an impact in the thermoelectric material science and especially in thermoelectric application scenarios.

Frank Pollman (MPI-PKS Dresden)

Dynamical signatures of quantum spin liquids

Condensed matter is found in a variety of phases, the vast majority of which are characterized in terms of symmetry breaking. However, the last few decades have yielded a plethora of theoretically proposed quantum phases of matter which fall outside this paradigm. Recent focus lies on the search for concrete realizations of quantum spin liquids. These are notoriously difficult to identify experimentally because of the lack of local order parameters. In my talk, I will discuss universal properties found in dynamical response functions that are useful to characterize these exotic states of matter.

Tomohiro Takayama (MPI Stuttgart)

Honeycomb iridate as a platform for topological spin liquid

Realization of quantum spin liquid, which may host novel topological order, has been a long-sought dream in condensed matter physics. Geometrically frustrated magnets with triangular motifs have been regarded as the most promising playground to search for spin liquids. Another route for a topological spin liquid was proposed by A. Kitaev [1], who showed that the ground state of honeycomb lattice with bond-dependent magnetic exchange is a gapless spin liquid. Implementing such magnetic coupling is, however, quite challenging in real materials.

Recently, honeycomb iridates emerged as a possible materialization of Kitaev spin liquid. In iridates, due to strong spin-orbit coupling of 5*d* Ir, the wave function of 5*d* electron is described by J_{eff} = 1/2 state [2]. The magnetic coupling between J_{eff} = 1/2 isospins in a 90-degree Ir-O-Ir bond (i.e. edge-sharing IrO_6 octahedra) was proposed to take the form of bond-dependent ferromagnetic coupling, invoking a possible route towards Kitaev spin liquid [3]. The honeycomb iridates a-Na_2IrO_3 and a-Li_2IrO_3, in reality, undergo antiferromagnetic ordering likely due to the presence of other magnetic interactions and lattice distortions [4]. In order to realize spin liquid ground state, development of new honeycomb iridates is highly desired.

By utilizing a topotactic ion-exchange reaction, we synthesized a new honeycomb iridate $H_3LiIr_2O_6$. $H_3LiIr_2O_6$ does not show any magnetic order down to 30 mK and the NMR measurements showed no signature of glass-freezing behavior despite large negative Curie-Wess temperature of ~-100 K. The finite susceptibility and specific heat down to the lowest temperature suggests that $H_3LiIr_2O_6$ has a gapless spin liquid ground state. By an application of magnetic field, the gapless ground state changes into a gapped spin liquid state. This behavior is in contrast to RVB-type spin liquid where magnetic fields are expected to reduce the spin singlet-triplet gap. In the talk, we will discuss the nature of spin liquid state and the relevance to the Kitaev model.

This work was done in collaboration with A. Kato, K. Kitagawa, Y. Matsumoto, R. Dinnebier, G. Jackeli and H. Takagi.

[1] A. Kitaev, Annals of Physics **321**, 2 (2006).

[2] B. J. Kim et al., Science **323**, 1329 (2009).

[3] G. Jackeli and G. Khaliullin, Phys. Rev. Lett. **102**, 017205 (2009).

[4] Y. Singh and P. Gegenwart, Phys. Rev. B **82**, 064412 (2010).