BEYOND! Materials Design and Discovery

abstract booklet

Ringberg, December 11-14th, 2016

Max Planck Institute of Microstructure Physics
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Aim of the Workshop

The workshop will focus on the design and discovery of novel materials with unique properties that could make possible advanced technologies, especially those concerned with information storage and processing, in the long-term.

The workshop will include both theoretical and experimental methods to accelerate the discovery of such materials, as well as the properties of the materials themselves.

Start | End Time

We invite you to arrive on Dec. 11th at Ringberg between 3-6 p.m. At that time rooms will be available for check-in and the registration will be open. On Monday you are invited to join a guided tour of the Castle by the manager Mr. Essl. He will show us around and provide us with some historical background information on the Castle and its secrets. Be curious! We end our Workshop on Dec. 14th. Check-out is foreseen after breakfast.

Address | Info on Accommodation

Schloss Ringberg - Schlossstraße 20 - 83708 Kreuth | Phone:+49 (0)8022 27 90 | http://www.schloss-ringberg.de/contact

The access code for internet access is available in the reception hall. Breakfast is served from 8:00 a.m. to 9 a.m.

Munich Airport ←→ Tegernsee Bahnhof (by Train/Taxi)

For your arrival/ departure by public transportation please check the time table of "Deutsche Bahn" at http://www.bahn.de/p_en/view/index.shtml and see attached time table to/ from Tegernsee. Make sure that you board the part of the train going to Tegernsee and not to Lenggries. Train will be split.

You can buy your ticket online, upon arrival at the vending machines or at the ticket counter before entering the S-Bahn area at the airport. Your destination is "Tegernsee Bahnhof" and the train ride takes approx. 2 hours.

Please use a taxi from the train station "Tegernsee" towards the castle. Taxi Kaufmann has a guest list and is informed about all arrival times that you have sent beforehand. You can reach the Taxi company by phone +49 (0)8022/ 5555 (code: MPI- Halle). For any questions you can contact Simone Jäger at +49 (0) 172/ 76.79.965.

We look forward to welcoming you at Ringberg. Have a save trip and see you soon.

Stuart Parkin

Towards Novel Dirac/Weyl Devices and Applications

| Dr. Mazhar Ali

Alexander von Humboldt Sofia Kovalevskaja Group Leader, MPI of Microstructure Physics, Halle | IBM Research, Almaden, Weinberg 2, 06120 Halle, Germany | maz@berkeley.edu

Recent discoveries of massless Dirac and Weyl fermions in a variety of materials have triggered a huge amount of experimental and theoretical interest from both chemists and physicists. Fantastic properties such as ultrahigh mobility, titanic magnetoresistance, and the chiral anomoly. Now, as thin-film growth of some of these materials is becoming more prevalent, interest is shifting into potential applications and devices based on these materials. Here we will show the novel transport properties of a new Dirac material, ZrSiS, as well as its potential in Fermitronic devices. Additionally, Dirac/Weyl materials will briefly be discussed in terms of their relation to spin hall angle as well as neuromorphic computing.

Biographical Sketch

Dr. Mazhar Ali pursued Bachelor's degrees in both Chemistry and Physics at the University of California, Berkeley before attending Princeton where he completed his PhD in Chemistry and Materials under Robert Cava. Here he studied Dirac and Weyl materials and discovered Titanic Magnetoresistance in WTe2. Afterwards, he went to IBM for a PostDoc under Stuart Parkin before accepting the Alexander von Humboldt Sofia Kovalevskaja Prize to begin his independent research group at the Max Plank Institute for Microstructure Physics in Halle.

From Bulk to Thin Films in Two Dimensional Transition Metal Dichalcogenides

| K. Gaurav Rana

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Two dimensional transition metal dichalcogenides (TMDs) have a renewed attention due to their rich variety of ground states ranging from metals to insulators, superconductors, topological insulators, Weyl semimetals. Possibility of tuning these properties in TMDs in their thin films or across their hetreointerfaces has made this field as one of the most attractive research directions. Recently, a semimetallic layered WTe2 has attracted considerable interest due to its peculiar non saturating large magnetoresistance (MR). It was found that WTe2 exhibits extremely large uniaxial magnetoresistance along the crystallographic c-axis [1], which is attributed to a balanced electron-hole resonance. Further, WTe2 is also predicted to be a Weyl semimetal. In this talk, first the evolution of electronic properties of exfoliated thin crystals of WTe2 from bulk to few nanometer regime is discussed. In addition, we focus on thermopower and Nernst measurements in WTe2, to probe the density of states (DOS) around the Fermi level which might have a role not only in observed large non saturating large MR but also predicted Weyl properties [2]. Using systematic MR measurements, we observe a negative MR in 1-Td WTe2 that can be attributed to chiral anomaly, predicted to exist for a Weyl semimetals. We also tune the Fermi level by electric field using back gate. Such investigations are extendable to other TMD heterostructures having tunable exotic properties. I will also discuss the growth of these 2 D materials, in particular epitaxially grown NbSe2 thin films using molecular beam epitaxy and impact of growth on the electronic properties is presented.

[1] Ali, M. N. et al. Large, non-saturating magnetoresistance in WTe2. Nature 514, 205–208 (2014).

[2] Chang, T. R. et al. Prediction of an arc-tunable Weyl fermion metallic state in MoxW1-xTe2. Nat. Commun. 7, 10639 (2016).

Biographical Sketch

I am a researcher in Prof. Stuart Parkin's group at Max Planck Institute of Microstructure Physics, Halle. I received my PhD in 2013 from Zernike Institute for Advanced Materials, University of Groningen, while working in the group "Physics of Nanodevices". I studied hot electron transport in complex oxide heterointerfaces, such as LSMO and SRO with Nb doped $SrTiO_3$ and hot electron spin transport across metallic spin valves.

I joined Prof. Parkin's research group in 2015. My research focuses are 1) Transitional metal dichacogenides and Weyl semimetals, 2) effect of ionic liquid gating in Mott insulators such as VO_2 and 3) Heusler materials such as Mn_2RhSn.

Recently, I have been investigating layered WTe_2 as ultra-thin exfoliated single crystals with thickness ranging from bulk like 100 nm to few monolayers. I am probing their electronic transport and thermoelectric behavior and tuning it using external stimuli such as large electric field generated by means of ionic liquid gating.

Topological Nonsymmorphic Metals from Band Inversion

| Lukas Muechler

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According to the Landau-Ginzburg paradigm, different phases of matter are distinguished by their symmetry. A recent major advance led to the recognition that insulators with the same symmetries and particle numbers can be topologically distinct. That is, for the same electron filling and symmetry class, one may have either trivial or topological insulators. This scenario is substantially modified for crystals having a broad class of spatial symmetries that are commonly found in nature called nonsymmorphic symmetries. Nonsymmorphic symmetries are fundamentally different, in that they naturally lead to energy bands that stick together, which guarantees that at certain fillings the phase of matter must *always* be gapless. Our work explores the distinct phases of matter within this broad class of spatial symmetries, but *for fillings that do not guarantee gaplessness*. We find that a topological phase transition separates a trivial, gapped phase from a topological, gapless phase. This contrasts with the conventional paradigm that a phase transition separates a trivial from a topological insulator. We show, based on ab-initio calculations and tight-binding models, that MTe_2 (M = W, Mo) monolayers without spin-orbit coupling are examples of this novel topological metal.

We further find that important aspects of the electronic properties of the MTe2 monolayer survive in bilayer and three-dimensional MTe2, which among other things show a record high magnetoresistance.We propose that the magnetoresitance has a unique topological origin - precisely, it originates from the topological metallicity discussed above.

Biographical Sketch

Lukas is a PhD student in the lab of Roberto Car in Princeton with an undergraduate degree from the University of Mainz in the lab of Claudia Felser.

His main interest is the theoretical study of topological phenomena in both interacting and non-interacting systems that lie in the intersection between Chemistry and Physics.

A big part of his work is concerned with symmetry protected topological phases and their classification, especially nonsymmorphic symmetries that can lead to novel topological phases in 2- and 3-dimensional crystals.

Additionally, Lukas tries to understand the physical and topological framework that underlies chemical theories, for example the distinction between aromatic and anti-aromatic compounds.

Berry phase effects in Heusler Compounds

| Jürgen Kübler, Claudia Felser, and Stuart Parkin

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In a short introduction the Berry phase and the anomalous Hall effect are explained under the assumption that the abelian theory suffices. For the case of the half-Heusler compounds we show our old graph that contains numerous topological insulators. Here fascinating ARPES results of the group support the band picture. GdPtBi, derived from the LnPtBi-group of the topological insulators, is an antiferromagnet with a non-vanishing anomalous Hall effect and outstanding topological properties, which are discussed. Turning to ferromagnetic half-Heusler, we pay a visit to the venerable PtMnSb speculating about the large Kerr effect in view of a peculiar property of the Berry-curvature. The full Heusler compounds lead us to Weyl Fermions that are shown not to be confined to semi metals, but also occur among the Heuslers, as was recently proposed by the Bernevig group in Princeton. The anomalous Hall effect in antiferromagnets of the related compounds Mn_3Ge, Mn_3Sn, and Mn_3Ir (hexagonal and cubic) finally supply more interesting cases to demonstrate the connection of the Berry curvature with topological properties, experimental and theoretical results supplying an enjoyable playground.

Biographical Sketch

After two years of studying Physics and Mathematics in Giessen, Jürgen Kübler spent five years as a Fulbright scholar in the USA, where he did complete his studies and received his doctoral degree. Before becoming a full professor at Technische Universität Darmstadt in 1981, he was a scientist at the Universities of Cologne, London, Bochum, the Fernuniversität Hagen and the Texas A & M University. He left for longer research stays that brought him to IBM's research centers in New York, Rüschlikon (Switzerland) and Oak Ridge (Tennessee, USA), as well as ETH Lausanne and the University of Illinois (USA). Its main work areas are the foundations of magnetism.

MBE growth and electronic tuning of Heusler thin films

| Chris Palmstrøm

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Heusler compounds are an exciting family of ternary intermetallics that can be composed of elements from a large fraction of the periodic table with their electronic properties being predicted to depend on the number of valence electrons per formula unit [1]. They have been predicted and experimentally shown to exhibit novel electronic and magnetic properties, such as half-metallic ferromagnetism [2] and semiconducting[3,4]. In general, Heusler compounds form two main variants: half-Heuslers (XYZ) with the $C1_b$ crystal structure and full-Heuslers (X_2YZ) with the $L2_1$ crystal structure. Although most half-Heusler compounds are expected to be topologically trivial, a number of half-Heusler compounds have been predicted to be topological non-trivial and should display topological surface states[5,6].

The half-Heusler compounds with composition XYZ can be thought of as being a zincblende structure of XZ with the Y atoms in the octahedral sites. The close similarity to the zincblende III-V compound semiconductors and the ability to adjust the lattice parameters of III-V semiconductors by alloying over the range of lattice parameters of many Heusler compounds, makes III-V semiconductors a good choice as substrates for Heusler compound epitaxial growth. Furthermore, molecular beam epitaxy (MBE) has been used to grow several full- and half-Heusler compounds on III-V semiconductors. PtLuSb is a half-Heusler compound that lies close to the normal to inverted band ordering transition with a zero-gap semiconducting band structure. Angle-resolved photoemission (ARPES) and spin-resolved ARPES are techniques ideally suited to investigate surface states and to determine if they are trivial or topological. This presentation will emphasize the MBE growth and integration of full- and half-Heusler compounds with III-V semiconductors as well as electronic tuning of trivial and non-trivial Heusler compounds.

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[5] H. Lin, L. A. Wray, Y. Q. Xia, S. Y. Xu, S. A. Jia, R. J. Cava, A. Bansil, and M. Z. Hasan, Nature Materials 9, 546 (2010).

[6] S. Chadov, X. Qi, J. Kuebler, G. H. Fecher, C. Felser, and S. C. Zhang, Nature Materials 9, 541 (2010).

Biographical sketch

Chris Palmstrøm is a Professor in the Electrical and Computer Engineering and the Materials Departments at the University of California, Santa Barbara. His research involves atomic level control and interface formation during molecular beam and chemical beam epitaxial growth of metallic compounds, metal oxides and compound semiconductors. He received his B.Sc. in physics and electronic engineering and Ph.D. in electrical and electronic engineering from the University of Leeds. After being a Research Associate at Cornell, he joined Bellcore as a Member of Technical Staff in 1985. From 1994-2007 he was a Professor in the Department of Chemical Engineering and Materials Science at the University of Minnesota and in 2004 became the Amundson Chair Professor. In 2007 he joined the faculty at the University of California, Santa Barbara. He has pioneered dissimilar materials epitaxial growth studies using a combination of molecular beam epitaxial growth with in-situ surface science probes including STM, XPS and AES, and ex-situ structural and electronic characterization.

An important aspect of his work has been to go beyond surface science and structural studies to make materials for device structures allowing for detailed electrical and optical measurements of materials and interfacial properties. Specific studies have emphasized metallization of semiconductors, dissimilar materials epitaxial growth, thin film analysis, and molecular beam and chemical beam epitaxial growth of III-V semiconductor heterostructures, Heusler compounds, metallic compounds, metal oxides, multifunctional, magnetic, thermoelectric, and spintronic materials, and superconductors. He is the author of over 250 publications. He is a Fellow of AVS, APS, and MRS. Some recent representative publications are:

1 *J. A. Logan, S. J. Patel, S. D. Harrington, C. M. Polley, B. D. Schultz, T. Balasubramanian, A. Janotti, A. Mikkelsen, and C. J. Palmstrøm, Observation of a topologically non-trivial surface state in half-Heusler PtLuSb (001) thin films, Nature Communications 7, 11993 (2016)*

2 *C. Liu, S. J. Patel, T. A. Peterson, C. C. Geppert, K. D. Christie, G. Stecklein, C. J. Palmstrøm, and P. A. Crowell, Dynamic detection of electron spin accumulation in ferromagnet-semiconductor devices by ferromagnetic resonance, Nature Communications 7, 10296 (2016).*

3 *C. J. Palmstrøm, Heusler Compounds and Spintronics, Progress in Crystal Growth and Characterization of Materials 62, 371 (2016).*

4 *B. Shojaei, P. J. J. O'Malley, J. Shabani, P. Roushan, B. D. Schultz, R. M. Lutchyn, C. Nayak, J. M. Martinis, and C. J. Palmstrøm, Demonstration of gate control of spin splitting in a high-mobility InAs/AlSb two-dimensional electron gas, Physical Review B 93, 075302 (2016)*

5 *S. J. Patel, J. K. Kawasaki, J. Logan, B. D. Schultz, J. Adell, B. Thiagarajan, A. Mikkelsen, and C. J. Palmstrøm, Surface and Electronic Structure of Epitaxial PtLuSb (001) Thin Films, Appl. Phys. Lett. 104, 201603 (2014).*

6 *J. K. Kawasaki, L. I. M. Johansson, B. D. Schultz, and C. J. Palmstrøm, Growth and transport properties of epitaxial lattice matched half Heusler CoTiSb/InAlAs/InP(001) heterostructures, Applied Physics Letters 104, 022109 (2014).*

Two-Dimensional Conjugated Polymers and Conducting Polymers: A New Paradigm for Optoelectronics

| Xinliang Feng

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Conjugated polymers are organic macromolecules which typically consist of one backbone chain of alternating double- and single-bonds. Thus conjugated polymers are usually defined as one-dimensional macromolecules with extended π-conjugation which exhibit unique electronic and opto-electronic properties. These conjugated polymers generally suffer from low charge carrier mobility, grain boundary and poor solid-state packing in comparison with their inorganic counterparts. Two-dimensional conjugated polymers can extend the conjugation of polymers from 1D to 2D. Thus, this provides the possibility to confront a major challenge facing linear polymer semiconductors. Sheet-like network can be regarded as n-strand ladder chains. In this respect, charge carriers can travel from one place to the other through different chains, and high charge carrier mobility can be expected. A first prominent example was already demonstrated by the extremely high carrier mobility of graphene – a prototypical 2D conjugated polymer from nature. Graphene can be synthesized either via top-down mechanical exfoliation or (electro) chemical exfoliation and bottom-up organic synthesis or chemical vapor deposition methods. Despite the exceptional physical properties associated with graphene, the lacking of bandgap prevents the integration of graphene in practical transistor applications.

In this lecture, we will present our recent efforts on the bottom-up synthetic approaches towards novel 2D conjugated polymers and conducting polymers with structural control at the atomic/molecular-level or at the meso-scale. In the first approach, solution synthesis of 2D conjugated polyphenylvinylene with carbon-carbon linkage will be presented. Such 2D polyphenylvinylene framework shows defined bandgap, reversible redox-behavior, few-layer feature and good solution processability. In the second strategy, we will demonstrate our latest development on the synthetic 2D conjugated polymers including 2D Schiff-base type covalent polymers and 2D metal-dithiolene/diamine coordination supramolecular polymers at the air-

water or liquid-liquid interfaces. The resulting 2D conjugated polymers exhibit single-layer feature, good local structural ordering and with a size of cm2. The functional exploration of such 2D single-layer conjugated polymers for the electrical and mechanical properties, as well as serving as efficient electrocatalytic water splitting catalysts will be demonstrated. Finally, we will present the supramolecular approaches to synergetic control the multi-component assembly, which results into 2D conducting polymers, such as polypyrrole and polyaniline nanosheets featuring 2D structures and with adjustable mesopores with/without on various functional free-standing surfaces. The unique 2D structures of these materials associated with tailored-made chemical structures and controlled bandgaps render them highly appealing for the development of next generation opto-electronic devices.

Nature. Comm. 2016, 7, 13461
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Nature. 2016, 531, 489
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Polym. Chem. 2016, 7, 4176
J. Am. Chem. Soc. 2015, 137, 14525
Nature Comm. 2015, 6, 8817
Angew. Chem. Int. Ed. 2015, 54, 12058
Adv. Mater. 2015, 27, 403

Biographical sketch

Xinliang Feng is a full professor at Technical University of Dresden. He received his Bachelor's degree in analytic chemistry in 2001 and Master's degree in organic chemistry in 2004. Then he joined Prof. Klaus Müllen's group at the Max Planck Institute for Polymer Research for PhD thesis, where he obtained his PhD degree in April 2008. In December 2007 he was appointed as a group leader at the Max-Planck Institute for Polymer Research, and in 2012 he became a distinguished group leader at the Max-Planck Institute for Polymer Research.

His current scientific interests include graphene, synthetic two-dimensional materials, organic conjugated materials, and carbon-rich molecules and materials for electronic and energy-related applications. He has published more than 280 research articles which have attracted more than 14000 citations with H-index of 60.

He has been awarded several prestigious prizes such as IUPAC Prize for Young Chemists (2009), Finalist of 3rd European Young Chemist Award, European Research Council (ERC) Starting Grant Award (2012), Journal of Materials Chemistry Lectureship Award (2013), ChemComm Emerging Investigator Lectureship (2014), Highly Cited Researcher (Thomson Reuters, 2014, 2015), Fellow of the Royal Society of Chemistry (FRSC, 2014).

He is an Advisory Board Member for Advanced Materials, Journal of Materials Chemistry A, and Chemistry -An Asian Journal. He is also one of the Working Package Leaders for European commission's pilot project Graphene Flagship.

Topological Orbital Ferromagnetism

| Yuriy Mokrousov

Topological Nanoelectronics Group, Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich, Germany | International Centre for Materials Science | y.mokrousov@fz-juelich.de

Since recently antiferromagnetic materials have become of great interest in spintronics owing to their insensitivity to external magnetic fields, strong response to applied electric fields, and a prospect of ultrafast dynamics of their staggered magnetization.

Remarkable properties of antiferromagnets are further enriched by their recently observed strong spin Hall response and its pronounced anisotropy. As a subclass of antiferromagnetic materials non-collinear antiferromagnets exhibit fascinating properties related to the observations that the non-trivial topology of real-space distribution of spins in latter compounds can give rise to various transport effects, for which the role of the spin-orbit interaction, traditionally viewed as the sole source of non-trivial geometry in reciprocal space, can be completely replaced by non-collinearity. In my talk, based on first principles theory, I will demonstrate that the effect of the chirality of non-collinear antiferromagnets does not only manifest in their sizeable Hall effect, but has crucial consequences for their orbital magnetism.

Taking for example such a classical respresentative of a non-collinear antiferromagnet as gamma-FeMn, I will show that it is the chirality of magnetic moments in the 3Q-state of this alloy, rather than spin-orbit interaction that gives rise to a sizeable orbital magnetization in FeMn. Given a close correlation of the orbital magnetization with the chirality of spins allows us to proclaim that gamma-FeMn belongs to a new class of materials which we refer to as "topological orbital ferromagnets" (TOFs), whose macroscopic magnetization is determined entirely by the orbital magnetism and whose properties are unaltered by spin-orbit interaction. The finite orbital magnetization in TOFs is a direct consequence of complex geometry of Bloch electrons in reciprocal space, which re-interpret the effect of chirality in real space as an effective magnetic field in k-space. Finally, I will present clear evidence that the TOFs can arise in two-dimensional geometry at surfaces of non-collinear magnets and as such go hand in hand with pronounced topological Hall effect and topological orbital magnetostriction -- properties, which make topological orbital ferromagnets unique building blocks in the emerging field of orbitronics.

Biographical Sketch

Prof. Yuriy Mokrousov works in the field of ab-initio materials research and phenomena discovery with strong emphasis on spin-orbit interaction effects in metals and insulators. Particular focus in his research falls on manifestation of geometrical and topological phases in complex magnetic materials associated with non-trivial Hall effects, spin-orbit torques, chiral magnetic interactions and chiral spin textures. He received his Ph.D. from RWTH Aachen University in Germany for his work in the area of density functional theory description of low-dimensional magnets done at the Institute of Solid State Research of Forschungszentrum Jülich. He did his postdoctoral research at the Peter Grünberg Institute of Forschungszentrum Jülich (with Stefan Blügel), Institute for Applied Physics of the University of Hamburg (with Stefan Heinze), and at the Physics Department of the University of California at Berkeley (with Ivo Souza). Since 2009 he is the leader of the Topological Nanoelectronics Group at the Institute for Advanced Simulation of Forschungszentrum Jülich. Since 2011 he is an Assistant Professor at the Physics Department of RWTH Aachen University.

Digital Foundry - Predicting New Materials and their Properties with Supercomputers

| Silvana Botti

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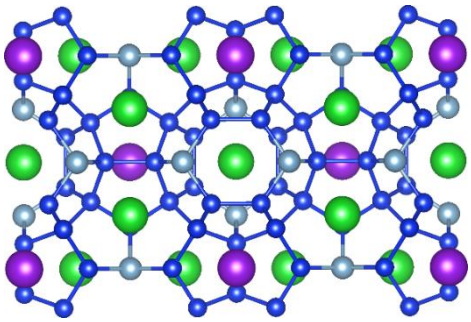
Can new materials with optimized properties be designed using supercomputers? In this lecture I will try to convince you through some examples from my recent work that first-principles calculations can efficiently speed up the discovery of new materials. Theoretical approaches based and going beyond density functional theory ally today accuracy and efficiency, and are therefore suitable tools for understanding the physics not only of simple perfect crystals, but also of nanostructured materials, doped semiconductors, interfaces, alloys, etc. As a result, *ab initio* simulations of spectroscopic properties can finally account for the complexity of "real" experimental samples, allowing accurate comparison of calculated and measured structural and excitation properties. The powerful combination of theoretical spectroscopy with high-throughput calculations and structural prediction can therefore provide a precious guide to experimentalists in the search of new materials. At present the systems we are interested in are varied, ranging from thin-films absorbers and transparent conductive oxides for solar cells, to thermoelectric materials and complex hydrides for on-board hydrogen storage.



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[5] Materials design on-the-fly, T.F.T. Cerqueira, R. Sarmiento-Pérez, M. Amsler, F. Nogueira, S. Botti, and M.A.L. Marques, J. Chem. Theory Comput. 11, 3955-3960 (2015).

[6] Identification of novel Cu, Ag, and Au ternary oxides from global structural prediction, T.F.T. Cerqueira, S. Lin, M. Amsler, S. Goedecker, S. Botti, and M.A.L. Marques, Chem. Mater. 27, 4562-4573 (2015).

Biographical sketch

Silvana Botti is Full Professor at the Friedrich-Schiller University of Jena, Germany. Born in Bergamo (Italy) in 1974, she obtains her PhD in 2002 at the University of Pavia in Italy. After working for two years as Marie-Curie Fellow at the Ecole Polytechnique in Paris, in 2004 she becomes Research Scientist at the French National Center for Scientific Research. In 2008 she moves to the University of Lyon. Since 2014 she holds the chair of Solid State Theory at the Friedrich-Schiller University of Jena. Her main research goal is to develop many-body treatments for theoretical spectroscopy combined with crystal structure prediction and high-throughput calculations, to design improved materials for specific applications. Her recent research activities focus on materials for energy production, storage and saving.

Topological Quantum Chemistry

| B. Andrei Bernevig

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I will present recent work completing the task of classifying all topological structures in a complete theory with tremendous predictive power. An implementation of our theory on the 230 space groups in nature reveals a wide range of new topological classes. We present a wide range of new topological insulators (>100) as well as ab initio results to support our claims.

Biographical sketch

B. Andrei Bernevig is a Eugene and Mary Wigner Assistant Professor of physics at Princeton University. He received his Ph.D. from Stanford University in 2006 on the Quantum Spin Hall effect. He performed his post-doctoral research at the Princeton Center for Theoretical Science from 2006-2009 working on Fractional Quantum Hall effect and topological phases as well as on the physics of iron-based superconductors. He joined the faculty at Princeton University in September 2009. His recent interests combine topological insulators, topological phases, fractional quantum Hall effect and iron-based superconductors.

Designing (Non-Composite) Room Temperature “Multiferroics”

| Jonathan Alaria

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Materials presenting multiple ferroic order (e.g. electric and magnetic polarisation) have the potential to be integrated in “Beyond CMOS” magnetoelectric disruptive technologies combining the advantageous properties of both ferroelectric and magnetic memories with fast switching speed and low power density. There has been significant progress in the fundamental understanding of magnetoelectric processes but a roadblock to translate this knowledge in useable devices lies in the lack of materials which possess the required properties at room temperature.

We have developed concepts to design such compound based on the perovskite structure. We have shown experimentally that it is possible to produce synthetic thin films of room temperature weak ferromagnet possessing a polar structure using isostructural perovskite blocks with the correct octahedral tilt combination. It is possible to extend this concept to bulk layered perovskite using crystal chemistry to engineer specific atomic displacements generating a polar structure and magnetization with a finite linear magnetoelectric susceptibility above room temperature. Another concept is based on constructing a percolating network of magnetic ions with strong superexchange interactions within a structural scaffold exhibiting polar lattice symmetries at a morphotropic phase boundary that both enhances polarization switching and permits canting of the ordered magnetic moments.

Biographical sketch

To date my work has focused on the growth of high quality single crystals or oriented/epitaxial thin films and the measurement of physical properties of novel magnetic materials. In particular, I have concentrated on three different classes of materials: (i) magnetic semiconductors, (ii) low dimensional magnets and (iii) multiferroics. I completed my Ph.D. in experimental physics in Prof. J.M.D. Coey group (Trinity College Dublin) and after a post-doctoral researcher position in the Department of Chemistry at University of Liverpool in Prof. M. J. Rosseinsky group I obtained a lectureship in the Stephenson Institute for Renewable Energy at University of Liverpool. I have developed specific skills in the growth of single crystals by chemical vapour transport and high temperature solution together with advanced electrical characterisation, with a focus on the correlation between electrical and magnetic properties by measuring Hall effect, magnetoresistance in large magnetic fields, and magneto-electric coefficient. I have been using neutron central facilities regularly to determine the magnetic and nuclear structure of complex inorganic materials.

Electronic Structure and Properties of a Few-Layer Black Phosphorus

| Mikhail Katsnelson

Institute for Molecules and Materials, Radboud University, Nijmegen, Netherlands | M.Katsnelson@science.ru.nl

I will review some theoretical issues related to a newly discovered two-dimensional material, few-layer black phosphorus (for the case of single layer, also known as phosphorene). This is a direct-gap semiconductor with a gap in Γ point changing from roughly 2 eV in single layer to 0.3 eV in the bulk, with anisotropic and essentially non-parabolic energy spectrum. I will present tight-binding parametrization of electron energy spectrum and its application to large-scale simulations of optical and plasmonic properties. At strong interlayer electric field (or potassium doping) electronic phase transition happens to semimetallic phase with anisotropic Dirac cones. I will discuss consequences of this transition for plasmon spectra and quantum Hall effect. I will also consider single- and two-phonon scattering processes and intrinsic limits on charge carrier mobility in single-layer black phosphorus which turn out to be much more restrictive than for graphene.

The talk is based on the works[1-8].

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Biographical sketch

Mikhail Katsnelson received his Ph.D. in 1980 in solid state physics from the Institute of Metal Physics (Ekaterinburg, Russia) where he stayed until 2001. After three years in Uppsala University, 2002-2004, M. Katsnelson became professor and head of the group of theory of condensed matter in Radboud University. His main scientific interests cover quantum many-body theory, electronic structure of solids, magnetism, graphene, pattern formation and self- organization in physical and chemical systems. M. Katsnelson is elected member of Royal Netherlands Academy of Arts and Sciences, Academia Europaea and Royal Society of Sciences at Uppsala.

Correlated Materials by Design

| Susanne Stemmer

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The control of phenomena caused by strong electron correlations via external electric and magnetic fields promises new applications in information processing and storage. Oxide heterostructures have emerged as new platforms to design, control, and understand phenomena caused by strong electron correlations. Compared to bulk materials, they offer precise control over dimensionality, control of lattice and orbital structure via strain, electrostatic doping, and the use of proximity effects to introduce different types of magnetic order. We will discuss these approaches using a specific interface system, namely the two dimensional electron liquid (2DEL) formed at interfaces between Mott insulating rare earth titanates and the band insulator $SrTiO_3$. Such interfaces exhibit a high-density 2DEL, of approximately ½ electron per surface unit cell, providing ~ 3×10^{14} cm^{-2} mobile charge. We will discuss the conditions for the emergence of electron correlation induced phenomena, such as unconventional metallic behavior, pseudogaps, and metal-insulator transitions in narrow quantum wells bound by two such interfaces, and their relation to the proximity to different types of magnetism and a quantum critical point. We will also discuss recent progress in the development of field effect devices and the degree to which they can be used to control these phenomena.

Biographical sketch

Susanne Stemmer is Professor of Materials at the University of California, Santa Barbara. She received her Diploma in Materials Science from the Friedrich-Alexander University Erlangen-Nürnberg (Germany). She did her doctoral work at the Max-Planck Institute for Metals Research in Stuttgart (Germany) and received her doctoral degree from the University of Stuttgart in 1995. Following postdoctoral positions she held an Assistant Professor appointment in Materials Science at Rice University from 1999 to 2002. In 2002, she joined the University of California, Santa Barbara. Her research interests are in the development of scanning transmission electron microscopy as a quantitative tool in materials science, novel dielectrics, oxide molecular beam epitaxy, and strongly correlated oxide heterostructures. She has authored or co-authored more than 220 publications. Honors include election to Fellow of the American Ceramic Society, Fellow of the American Physical Society, Fellow of the Materials Research Society, Fellow of the Microscopy Society of America, and a Vannevar Bush Faculty Fellowship.

Theory of Spin-Orbit Induced Magnetic Phenomena in Solids

| Peter Oppeneer

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The relativistic spin-orbit interaction is responsible for a variety of interesting magnetic phenomena in condensed matter physics, such as the magneto-crystalline anisotropy and the magneto-optical Kerr and Faraday effects. Here I focus on spin-orbit-related phenomena that have recently drawn attention. One of these is the appealing possibility to use short pulses of circularly polarized laser light to induce magnetization in metals and thus achieve all-optical helicity dependent magnetization switching. Combining 2nd order density matrix theory with *ab initio* calculations we provide materials' specific predictions of the amount of induced magnetizations, and demonstrate a surprising difference between induced spin and orbital magnetizations. On the basis of the Dirac-Kohn-Sham equation we show further the existence of a new relativistic coupling term which linearly couples the optical angular momentum of the electro-magnetic field to the electron's spin. Also, we address the importance of ultrafast relativistic spin-flip processes that can be created by optical excitation or electron-phonon scattering and that have been proposed to explain ultrafast laser-induced demagnetization. Lastly, we provide a rigorous derivation for the origin of the Gilbert damping in the Landau-Lifshitz-Gilbert equations of spin dynamics, which we show to contain an isotropic Gilbert contribution as well as anisotropic Ising-like and chiral Dzyaloshinskii-Moriya-like contributions.

Biographical sketch

Peter Oppeneer studied theoretical physics in Utrecht and Amsterdam (PhD), the Netherlands. During his postdoctoral research stay with Prof. J. Kübler at the TU Darmstadt (1988-1992) he became interested in developing theory for spin-orbit-interaction induced magnetic phenomena in solids such as the magneto-optical Kerr effect. He continued to investigate relativistic effects in valence band and X-ray spectroscopy of correlated materials at the TU Dresden, where he did his habilitation. After being staff researcher at the IFW Dresden and Priv. Doz. at the TU Dresden, he became professor at Uppsala University, Sweden, where he develops theory for, among others, ultrafast laser-induced demagnetization and spin currents, unconventional superconductivity, relativistic electron-phonon spin-flip scattering processes, and for spin-relaxation mechanisms of spin dynamics.

Design and Discovery of Engineering Materials from First Principles

| Jörg Neugebauer

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Modern engineering materials have evolved from simple single phase materials to nano-composites that employ dynamic mechanisms down to the atomistic scale. The structural and thermodynamic complexity of this new generation of structural materials presents a challenge to their design since experimental trial-and-error approaches, as successfully used in the past, are often no longer feasible. Ab initio approaches provide perfect tools to new design routes but face serious challenges: Free energies of the various phases are almost degenerate, requiring theoretical formalisms that accurately capture all relevant entropic contributions. In addition, their hierarchical nature with respect to length and time makes them challenging for any atomistic approach. Combining accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts enables us to address now these issues and to determine free energies and derived thermodynamic quantities that often rival available experimental data. The flexibility and the predictive power of these approaches and the impact they can have on the development of new strategies in materials design and discovery will be discussed for examples ranging from metallic alloys with superior mechanical properties to optoelectronic and high-power electronic devices.

Biographical sketch

Prof. Dr. Jörg Neugebauer is Director and Executive at the Max-Planck-Institut für Eisenforschung GmbH in Düsseldorf, Germany. His research fields include theoretical solid state physics, multiscale simulations, ab initio thermodynamics, quantum mechanics and electronic structure theory. He received his diploma and PhD degree from the Humboldt University Berlin, Germany, in 1987 and 1989, respectively. Subsequently he went as visiting scientist to the Fritz-Haber Institute in Berlin (until 1993) and to the XEROX Palo Alto Research Center (until 1996). In 1998 he became head of an independent Max-Planck-Research group (C3), and in 2003 Professor (C4) at the University of Paderborn. Currently, he is heading the department of Computational Materials Design in the Max-Planck-Institut für Eisenforschung. He is a Scientific member of the Max-Planck-Society, Elected Member of the Academy of Sciences and Art in North Rhine-Westphalia, Elected Chair of the Metals and Materials (MM) Division of the German Physical Society (DPG), Chairman of the expert committee “Digital transformation in materials engineering” of the Association of German Engineers (VDI), Professor at the University of Paderborn, Honorary Professor at the Ruhr-Universität Bochum and Director of the Advanced Study Group “Modeling” at ICAMS.

Electron Correlations in Magnetic Materials

| Alexander Lichtenstein

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Effects of electron interactions in magnetic materials, oxides and transition metals will be discussed. Modern density functional theory describes well the ground state properties for moderate correlated metals, but failed for some Mott insulators. Spectroscopy of strongly correlated magnetic materials with transition or rare-earth elements can be well incorporated only in correlated electronic structure scheme. We introduce a multi-orbital spin-polarized dynamical mean field theory which allowed investigating the correlations effects in real materials. Prospects of realistic description of itinerant magnetism in transition metals and Mott insulators state in complex oxides will be discussed.

Biographical sketch

Alexander I. Lichtenstein studied at the University of Yekaterinburg and received his doctoral degeree in 1982. He was then employed at the *Institute of Solid State Chemistry* in Ekaterinburg. From 1989 he worked at the *Max Planck Institute for Solid State Research* in Stuttgart and from 1995 onwards at *Forschungszentrum Jülich*. In 1998 he became Professor of Theoretical Physics at Radboud University in Nijmegen and since 2004 he is professor in Hamburg. He is Head of the group Magno *The Theory of Magnetism and Electronic Correlations*. The main research activities of his group are related with fundamental quantum aspects of spin phenomena in nanomagnetic structures. Formation of local spin and orbital magnetic moments, effective exchange interactions as well as different spin, charge and orbital ordering depends crucially on the electronic structure of real nanosystems.

Learning Descriptors from Materials-Science (Big) Data

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Scientific discoveries often proceed from the accumulation of consistent data to the identification of functional dependencies among the data, i.e., a model that is able to predict yet unseen phenomena. Ultimately, a theory may be constructed to explain the model with few simple principles. Classical examples are i) the three laws of Kepler, that were empirically found by observing the known data on the solar system, later justified by Newton's theory of gravitation, and ii) the periodic table of Mendeleev, empirically constructed from data on the chemistry of known elements, later justified by the atomic theory within quantum mechanics.

In the last decades, statistical learning has been developed in order to find optimal and stable functional dependencies among data, in particular when some ancillary knowledge can be formalized and included in the search for optimal solutions.

We present a recently introduced compressed-sensing based methodology and its latest extension, for the identification of functional dependencies where the descriptor (the set of input variables of the functional dependence) is selected out of a dictionary of "well formed" candidate analytical expressions. Such candidates are constructed as non-linear functions of a set of basic "physically meaningful" features, called primary features.

Furthermore, we present a complementary method, called subgroup discovery (SGD), designed for constructing statements, in the form of true/false boolean expressions, about an optimal subset of candidate functions of primary features.

Results from the application of both methods are presented for the crystal structure prediction of binary materials and (only for SGD) for the identification of relationships between electronic- and atomic-structure properties of metal nanoclusters.

Biographical sketch

Since 2011, Luca M. Ghiringhelli is a group leader at the Fritz Haber Institute of the MPG, in the theory group led by Prof. Matthias Scheffler. His background is in computational statistical mechanics and electronic structure methods, applied for the evaluation of thermodynamic and kinetic properties of bulk materials, surfaces, and nano-clusters. Recently, he started applying methods inspired to compressed sensing to the modeling of big data in materials science.

Scientific Curriculum

2005-2008 PostDoc at Max Planck Institute for Polymer Research (Mainz), Theory Department

2006 Dr. rer. nat., Universiteit van Amsterdam, Van't Hoff Institute for Molecular Science

Since 2008 Staff Member at the Fritz Haber Institute of the Max Planck Society, Berlin

Major Research Areas

Configurational sampling of transition metal nanoclusters and comparison with experiments via vibrational analysis.

Development of accelerated schemes for the efficient sampling of the configurational space of atomic clusters.

Thermodynamics of metal clusters in a realistic atmosphere of ligands (finite temperature and pressure).

Challenges in Engineering Exotic Spin-Liquid Materials

| Maria-Roser Valentí

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The realization of a Kitaev spin liquid appears to represent a very significant synthetic challenge. In this talk we shall revisit the magnetic interactions and excitations in some proposed candidates for Kitaev physics like hexagonal iridates and RuCl$_3$ by a combination of ab initio density functional theory calculations and microscopic model considerations. From this analysis we will discuss the potential for realizing exotic spin liquid phases in real materials.

Biographical sketch

Prof. Roser Valenti's expertise is the microscopic modelling of strongly correlated materials by a combination of ab initio techniques and many-body methods. Her field of reseach includes unconventional superconductors, frustrated magnetism, oxide heterostructures, and topologically-non-trivial phases. She received her Ph.D. from the University of Barcelona for her work on variational wavefunctions for low-dimensional quantum spin systems. She did postdoctoral stays at the University of Florida in Gainesville, the TU Dortmund and the University of Saarland where she was awarded a Heisenberg fellowship.

Controlling Band Structure and Electronic Correlations by Dimensional Confinement and Epitaxial Strain in Quantum Materials

| Kyle Shen

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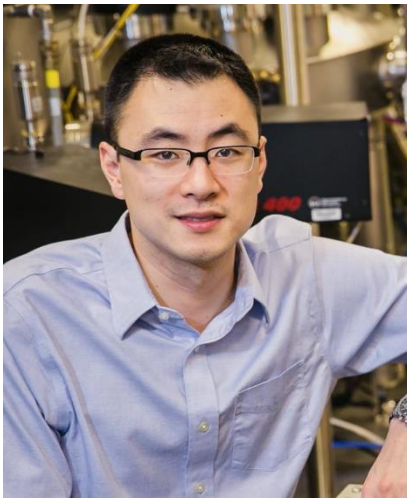
Our ability to control the electronic structure of materials, for instance at semiconductor interfaces, has had enormous scientific and technological implications. Recently, this concept has been extended to materials which possess inherently strong quantum many-body interactions, such as strongly correlated transition metal oxides, allowing us to synthesize artificial heterostructures which can harbor novel electronic or magnetic properties. The ability to deterministically manipulate the strength of electron correlations or the electronic band structure will be critical to designing new materials with novel properties. I will describe some examples of our recent work in thin films of nickelates, iridates, and ruthenates, and how we have used both epitaxial strain as well as dimensional confinement in atomically thin films to control the strength of electronic correlations, the electronic band structure, the Fermi surface topology, and drive a metal-insulator transition. These new insights could someday enable deterministic control over the emergent properties of quantum materials.



Biographical sketch

Kyle Shen is as Associate Professor of Physics at Cornell University. He received his undergraduate degrees in Physics and Electrical Engineering at the Massachusetts Institute of Technology, and his Ph.D. in Applied Physics from Stanford University. His research interests are in controlling the properties of correlated quantum materials, such as unconventional and high-temperature super-conductors, metal-insulator transitions, and magnetic materials, using a combination of molecular beam epitaxy and angle-resolved photoemission spectroscopy.

Engineering Topological Phases in Coupled Wire and Coupled Plane Systems

| Jelena Klinovaja

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I will discuss low-dimensional condensed matter systems, in which topological properties could be engineered on demand. I will focus on 'strip of stripes model' consisting of weakly coupled one-dimensional wires [1-3], where interaction effects in the wires can be treated non-perturbatively via bosonization. First, I will focus on two-dimensional anisotropic systems. Such systems can exhibit the integer or fractional quantum Hall effect, quantum spin Hall effect as well as anomalous quantum Hall effect. The bulk gap can be opened not only by tunneling between wires [1-3] but also by periodic driving with applied electric fields [4]. The latter case is described within the Floquet formalism [4]. I will then present the extension to three-dimensional systems based on weakly coupled planes which exhibit topological phases [5].

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Biographical sketch

Jelena Klinovaja received her Bachelor and Master degree in Applied Mathematics and Physics from the Moscow Institute of Physics and Technology (State University), Department of General and Applied Physics, in 2007 and 2009, resp. Subsequently, she joined the group of Prof. Daniel Loss at the University of Basel, where she received her PhD in Theoretical Physics in 2012 with summa cum laude. In 2013, she was awarded a three-year Harvard Fellowship to perform independent research in the area of the theoretical quantum condensed matter physics. Klinovaja was appointed as a tenure track assistant professor at the Department of Physics at the University of Basel in 2014. In her career, she was offered several prestigious fellowships and received research prizes such as the Swiss Physical Society Prize 2013 in Condensed Matter Physics, sponsored by IBM.

Notes