

Multiorb 2011 – Multiband and Multiorbital Effects in Novel Materials

International Summer School, Cargèse, France, August 1-13, 2011

Final Report

Organizers: *Peter Hirschfeld* – Univ. Florida, FL, USA
Ricardo Lobo – ESPCI-ParisTech, CNRS, UPMC, Paris, France
Marino Marsi – Univ. Paris-Sud, Orsay, France
Ilya Vekhter – Louisiana State Univ., LA, USA

1. Summary

The past few years has seen a myriad of new phenomena involving multiorbital and multiband effects on condensed matter systems. These effects represent a bowl of fresh air in a field that has been dominated by strongly correlated electronic effects on a single band picture such as cuprates and transition metal oxides. Iron based superconductors are materials where superconductivity emerges from an interplay and communication of several bands at the Fermi level. Manganites present an orbital interconnection with charge carriers motion that leads to fascinating effects including metal insulator transitions and colossal magnetoresistance. The effects of coexisting light and heavy quasiparticles in heavy fermion materials still produce unexplained phenomena such as the unknown nature of the order parameter observed in URu₂Si₂. The connection of surface states and bulk electronic bands may create topologically protected conducting states, with remarkable properties, in an otherwise simple semiconductor. Multiband and multiorbital effects highlight the competition and coexistence of otherwise exclusive phenomena, such as magnetism and superconductivity. In our current perspective of condensed matter physics, it is paramount to include these multiband and multiorbital effects to develop a comprehensive understanding of a variety of correlated systems.

In this scenario we organized a summer school at the "Institut d'Études Scientifiques de Cargèse" in Corsica, France. The school was aimed at bringing to junior scientists, entering the correlated electron community, novel and exciting experiments, theory, and phenomenology of multiorbital/multiband condensed matter systems. In order to keep the novelty of the field in perspective, and facilitate the understanding of these phenomena, we also set several presentations to fundamental, basic physical principles.

The school covered a wide variety of topics related to multiband and multiorbital effects, such as multiband superconductivity; phase competition and/or separation; exciton condensates; orbital ordering; orbital currents; orbital selective metal-insulator transitions; and protected topological states. These phenomena were discussed in various systems including pnictides and chalcogenide iron based superconductors, cobaltates, manganites, graphene, Mott insulators, topological insulators, and others. The school dealt with the most advanced theoretical methods for the study of these issues, along with a selection of different experimental approaches (such as scanning tunneling microscopy and spectroscopy, photoelectron spectroscopy, ultrafast spectroscopy) used to probe this new exciting physics. In honor of the 100th anniversary of the discovery of superconductivity the school was closed with a vivid round table on the subject.

The school was set in a format that allowed for longer pedagogical lectures, more recent research talks and contributions from the participants. We also had "wiki" sessions (described in more detail in the next section) that allowed for a strong interactive participation of the school attendants. The majority of the school participants were PhD students and post-docs, coming mostly from European and North American countries.

2. Scientific content and discussions

Presentations at the school were given in different ways aiming at different perspectives. Here we report each kind of presentation, its purpose and its outcomes. Copies of the presentation slides are available at the school web site:

<http://chercheurs.lps.u-psud.fr/multiorb2011/>

2.1. Lectures

Lecturers were allotted two or three 50 minutes slots, which included 15 minutes for discussions. We specifically asked for these lectures to be pedagogical and for intervenants to use at least 2/3 of their time to present a broad overview of the field, not their particular research. The vast majority of the speakers followed these guidelines which lead to a large participation of the audience in the discussion portion of the lectures. In the following we describe the specific lectures presented at the school.

Thomas P. Devereaux – Stanford University – gave introduced the theory of Fe-based superconductors in three lectures. These lectures covered the main differences in the chemistry of Fe in different materials and stressed the importance of their multiband character in calculating superconducting properties which allow for exotic phenomena such as pairing from repulsive interactions.

Johnpierre Paglione – University of Maryland – presented two lectures introducing the current experimental scenario of Fe-based superconductors. He stressed the interplay of structural, magnetic and superconducting states. This overview covered efforts in the growth and characterization of new compounds, as well as key experimental observations.

Dmitri N. Basov – Univ. California San Diego – showed the information provided by the optical conductivity on Fe-based superconductors. In particular he made a parallel between pnictides and cuprates, stressing similarities and differences between these materials.

Jennifer Hoffman – Harvard University – covered the state of the art STM results on Fe-based materials in her two lectures. She made a thorough introduction on the technique highlighting its strength and shortcomings. She showed how STM probes multiband effects and gives information on the gap symmetry.

Adam Kaminski – Iowa State University – presented two lectures on Angle Resolved Photoemission Spectroscopy (ARPES) on Fe-based superconductors. He showed how to measure the complex band structure of this materials and the information that can be obtained on the superconducting gap.

Jean-Pascal Brison – CEA/UJF Grenoble – made a comprehensive review on multigap superconductivity in three lectures. He introduced the extension of BCS theory to account for multiple bands and gave multiple examples on prototypical two band superconductor MgB_2 .

Jörg Schmalian – Institut für Technologie Karlsruhe – presented three lectures on graphene physics. He showed how the band structure is calculated and the importance and novelty of the Dirac cones. He extended the discussion to electron-electron interaction effects, quantum critical effects and ultrafast effects.

Shou-Cheng Zhang – Stanford University – had three lectures on Topological insulators, new states of quantum matter which have topologically protected gapless states due to surface effects.

Jérôme Lesueur – ESPCI – two lectures covered the physics of two dimensional electron gas physics at SrTiO₃ interfaces. These are systems where the interface of two insulating materials develops a 2D conducting system. He covered the orbital arrangements at the interface, which combined with the quantum paraelectric behavior of SrTiO₃, leads to a phase diagram where electronic orders (superconductivity, magnetism, orbital orders) may appear.

Jeroen Van Den Brink – IFW Dresden – gave three lectures on orbital degrees of freedom in strongly correlated transition metal compounds. He presented a very pedagogical introduction to open d-shell systems, spin and orbital degrees of freedom, strong electronic correlations, Hubbard U and Hund J evolving afterwards to more complex physics such as compass models and relativistic spin-orbit coupling.

Cristian Batista – Los Alamos National Laboratory – had two lectures on orbital effects in frustrated Mott insulators starting from a single band picture and moving into how multi-orbital physics emerges from singleorbital Hubbard models.

Daniel Agterberg – Univ. Wisconsin – gave 3 lectures on superconductivity without parity symmetry where the role of breaking parity symmetry is much less well understood than the role of breaking time reversal symmetry. He also covered 2D interface electronic gases and topological insulators.

Matthias Vojta – Technische Universitaet Dresden – had three lectures on orbital-selective Mott transitions, where conduction electrons undergo a partial Mott localization.

Peter Littlewood – Argonne National Laboratory – three lectures covered the condensation of excitons and polaritons, where a dense system of electrons and holes would be unstable toward an excitonic (electrical) insulator. He covered several aspects of exciton formation in semiconductors, as well as its consequences in terms of BCS to BEC crossover; open system dynamics and decoherence; and quantum dynamics.

2.2. Scientific Talks

A second kind of presentations covered more cutting edge results and consisted of up-to-date scientific talks. The speakers were given 60 minutes out of which 15 were allotted for discussions. These talks came in complement to the overview and more introductory presentations by the lecturers.

Elena (Leni) Bascones – Instituto de Ciencia de Materiales de Madrid – talked about iron pnictides as multiorbital antiferromagnets. She covered the on going debate on the origin of magnetism opposing the itinerant (weak coupling) versus localized (strong coupling) nature of magnetism and stressed the importance of Hund's coupling.

Florence Rullier-Albenque – CEA-Saclay – talked about multiband description of the transport properties in the iron pnictides. She presented a vast set of results covering different families of pnictides and how the transport relates to the presence of multiple bands in the system.

Jure Demsar – University of Konstanz – talked about the information ultrafast femtosecond time-resolved spectroscopic techniques can bring to study multi-

component order parameter dynamics. He covered various systems, from conventional BCS low-Tc superconductors to multi-gap pnictide high temperature superconductors.

Véronique Brouet – Université Paris-Sud – covered new types of electronic orderings in layered cobaltates from an ARPES stand point. She discussed how close (or how far) are these systems from a Mott insulator.

Girsh Blumberg – Rutgers – talked about Raman spectroscopy of multiband superconductors, in particular MgB_2 and pnictides. He discussed how Raman showed multiple gaps in multiband systems and its effects on the order parameter.

Henri Alloul – Université Paris-Sud – dealt with NMR study of the pressure induced Mott transition to Superconductivity in the newly discovered Cs_3C_{60} isomeric compounds.

Silke Biermann – Ecole Polytechnique – talked about effective orbital degeneracy (and reduction thereof) in correlated systems. She dealt with the Mott transition in multi-orbital Hubbard models, with particular emphasis on the interplay of crystal field splitting and correlation effects.

Natalia Perkins – Univ. Wisconsin-Madison – talked about quasi one-dimensional magnetism in vanadium oxides, stressing geometrically frustrated magnets with orbital degeneracy. She discussed how the interplay between spin, orbital and lattice degrees of freedom leads to a variety of interesting ground states and elementary excitations.

Roser Valenti – Goethe University Frankfurt – talked about frustration and multiorbital effects in Mott insulators and superconductors from an *ab initio* perspective.

Hae-Young Kee – University of Toronto – covered the nematic quantum critical point in multi-orbital systems. In particular she made an extensive presentation on ruthenates and their relation to multi-orbital materials.

Daniel Khomskii – Universitaet zu Koeln – talked about charge transfer systems and oxygen holes paying a special attention to the role of p-electrons (oxygens) in the case of small or negative charge transfer gap.

2.3. Contributed talks

We also reserved time in the program for contributed talks from the school participants. These talks were chosen during the school from the posters presented. There were three contributed sessions each with three 20 minutes presentations.

2.4. Wiki sessions

In order to promote a large participation of all school attendants we reserved four time slots for "wiki" sessions, roughly at the end of every other day. We established an interactive web site where attendants could post, anonymously, questions, comments or requests for further discussion concerning the subject of the preceding talks and lecturers. We then asked for volunteers amongst the participants to host the session. These volunteers had the task of reading and trying to come up with an answer to the posted comments. They typically had an afternoon's time to prepare the session. During the session they presented their thoughts on the problem as a starting point for a discussion with the audience and feed back from the speakers.

Each wiki session was hosted by about 5 attendants and addressed 6 to 10 questions. These sessions were very well perceived by both attendants and lecturers/speakers. The attendants who hosted the sessions did a very good job in preparing their thoughts on the questions posted, which promoted a very good exchange with the whole audience. Some of the speakers also posted answers to some of the queries on the wiki page.

2.5. Round table

In honor of the 100th anniversary of the discovery of superconductivity we closed the school with a round table on the subject. This table was hosted By Peter Littlewood (Argonne National Lab.) and Henri Alloul (Univ. Paris-Sud). Prior to the session we asked all school participants to post on the wiki page questions and subjects they would like to see discussed on this round table. At the session, both hosts made a short presentation on their views on superconductivity and then proceeded to a discussion with the audience where they tried to address the comments posted on the web page.

3. Assessment of the results

As a whole the vast majority of the lecturers made a large effort to follow the school guidelines. The presentations were very clear and pedagogical. In our organization of the schedule, we had allotted lectures of 35 minutes followed by 15 minutes for discussion. This is a very long time for discussion compared to the lecture length and one might expect long silent moment in the discussion. It turned out that in most cases 15 minutes were not long enough and the discussion progressed afterwards in the free time. This was a consequence of lectures prepared with a proper amount of introductory material and overview of the field. Most lecturers made a large effort to avoid presenting her/his results alone and really covered a big picture in their respective fields.

Scientific talks were asked to be more cutting edge results but still have enough introductory material to allow for the whole audience to follow at least part of the subject. These talks had a 45+15 minutes format and, once again the discussion time was completely filled. And, again, the majority of the speakers made an effort to cover their subject in an accessible way for the school attendants.

Virtually all school attendants presented a poster which was discussed over two afternoon sessions. These poster sessions were the basis for the choice of contributed talks. These contributed speakers were chosen with a very short notice (24-48 hours before the contributed session). Nevertheless, the attendants took up the challenge and gave nice presentations on their respective works.

The "wiki" sessions turned out to be a very nice surprise. The attendants who hosted the sessions did a wonderful job in addressing the questions asked on the web page and promoting a large discussion during the session. We had a very positive feedback on the format of these sessions, both from the school attendants and the lecturers/speakers. The possibility of posting anonymous questions on the web page was also appreciated. It allowed for the participation of attendants who did not feel comfortable asking a question during a lecture or a talk. At the end of the school there were over 60 entries in the wiki web page.

The closing round table also benefited from the wiki page as several questions were posted before the session. This allowed for the round table hosts (and all school participants, in fact) to think about the issues and have a better view of what to discuss during the session.

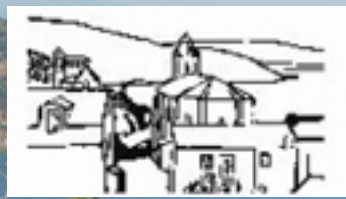
The only negative feed back we had concerned free time. Several school attendants missed more free time for one to one discussions with other attendants and school lecturers and speakers. We had 2–3 hours evry day for this sort of exchange, but a little bit more time would have been well received. This problem was partially smoothed by the fact that most lecturers and speakers did follow the organizers' request to stay on site for at least one week.

Let us close this repport with some administrative remarks.

The school was attended by 43 participants (out of which 23 are from Europe and 14 from North America) in addition to 25 speakers and lecturers (out of which 14 are from Europe and 11 from North America) and the 4 organizers. The organizing committee decided to give minimum travel support and cover the local expenses for almost all the participants. This allowed us to have a large number of young researchers attending the school.

The financial support for the school came from ICAM, Intelbiomat and Triangle de la Physique. The CNRS support the school through the work and logisitc provided at l'Institut d'Études Scientifiques de Cargèse (IESC).

All administrative tasks as well as a large part of the local logisitcs, was wonderfully carried out by Nadine Mehl (Univ. Paris-Sud) who worked in close relation with the local IESC staff.



Multiorb 2011

Multiband and Multiorbital Effects in Novel Materials
August 1-13, 2011

Multiband and Multiorbital Effects in Novel Materials

The school will be held at the Institut d'Etudes Scientifiques de Cargèse,
Corsica, France - August 1-13, 2011

Organizing committee:

Peter Hirschfeld, University of Florida, USA
Marino Marsi, Université Paris-Sud 11, FR
Ricardo Lobo, ESPCI-ParisTech, France
Ilya Vekhter, Louisiana State University, USA

Advisory committee :

H. Alloul , Université Paris-Sud 11, FR
P. Littlewood, University of Cambridge, UK

Invited Lecturers :

D. Agterberg, Milwaukee, WI
H. Alloul , Orsay, France
E. Bascones, Madrid, Spain
D. Basov, San Diego, CA
C. Batista, Bariloche, Argentina
S. Biermann, Palaiseau, France
G. Blumberg, Rutgers, NJ
J.-P. Brison, Grenoble, France
V. Brouet, Orsay, France
J. Demsar, Constance, Germany
T. Deveraux, Stanford, CA
J. Hoffman, Harvard, MA
A. Kaminski, Ames, IA
H.Y. Kee, Toronto, Canada
D. Khomskii, Loughborough, UK
J. Lesueur, Paris, France
P. Littlewood, Cambridge, UK
J. Paglione, Maryland, MD
N. Perkins, Madison, WI
F. Rullier-Albenque, Saclay, France
J. Schmalian, Karlsruhe, Germany
R. Valenti, Frankfurt, Germany
J. van den Brink, Leiden, Netherlands
M. Vojta, Dresden, Germany
S.-C. Zhang, Stanford, CA



Multiband and Multiorbital Effects in Novel Materials

The school will be held at the Institut d'Etudes Scientifiques de Cargèse, Corsica, France August 1-13, 2011

SCOPE OF THE SCHOOL

Among the many emergent phenomena in correlated electron systems, Multiband and Multiorbital Effects are currently attracting a lot of interest worldwide.

The discovery and exploration of Fe-based superconductors over the last two years is only the latest example of the rich physics of multiband/multiorbital correlated metallic systems. In a wide variety of compounds, from topological insulators and doped semiconductors to manganites and heavy fermion superconductors, the interplay between orbital/band degrees of freedom and quasiparticle motion is an essential component for a comprehensive understanding of the correlated system. The goal of the school is to provide a comprehensive overview of the experimental manifestations of this behavior and connections between different measurements, routes to uncovering the physics behind them, and theoretical tools to address these phenomena. The school is aimed at research-active graduate students and postdocs.

The workshop is sponsored by ICAM, the Institute for Complex Adaptive Matter (<http://www.i2cam.org/>).

	Mon 8/1	Tue 8/2	Wed 8/3	Thu 8/4	Fri 8/5	Sat 8/6	Sun 8/7
9am		Registration breakfast + Introductory remarks 8:30am - 10:30am	vd Brink II 9am - 9:50am	Zhang II 9am - 9:50am	Zhang III 9am - 9:50am	Hoffman I 9am - 9:50am	
10am			Batista II 9:50am - 10:40am	vd Brink III 9:50am - 10:40am	Schmalian II 9:50am - 10:40am	Kaminski I 9:50am - 10:40am	
11am		vd Brink I 10:30am - 11:20am	Coffee 10:40am - 11:10am	Coffee 10:40am - 11:10am	Coffee 10:40am - 11:10am	Coffee 10:40am - 11:10am	
12pm		Batista I 11:20am - 12:10pm	Paglione II 11:10am - 12pm	Schmalian I 11:10am - 12pm	Basov I 11:10am - 12pm	Schmalian III 11:10am - 12pm	
1pm		Lunch 12:10pm - 1:45pm	Lunch 12pm - 1:45pm	Lunch 12pm - 1:45pm	Lunch 12pm - 1:45pm	Lunch 12pm - 1:45pm	
2pm		Devereaux I 1:45pm - 2:35pm	Devereaux II 1:45pm - 2:35pm	Vojta II 1:45pm - 2:35pm	Perkins 1:45pm - 2:45pm	Basov II 1:45pm - 2:35pm	
3pm		Paglione I 2:35pm - 3:25pm	Bascones 2:35pm - 3:35pm	Devereaux III 2:35pm - 3:25pm	3 contributed talks 2:45pm - 3:45pm	Blumberg 2:35pm - 3:35pm	
4pm		Break 3:25pm - 5:30pm	Break 3:35pm - 6pm	Poster ads 3:25pm - 4:20pm	Break 3:45pm - 6pm		
5pm				Poster session 4:20pm - 7:30pm			
6pm		Rullier-Albenque 5:30pm - 6:30pm					
7pm		Vojta I 6:30pm - 7:20pm	Zhang I 6pm - 6:50pm		Vojta III 6pm - 6:50pm		
8pm			Wiki 6:50pm - 7:50pm		Wiki 6:50pm - 7:50pm		

	Mon 8/8	Tue 8/9	Wed 8/10	Thu 8/11	Fri 8/12	Sat 8/13	Sun 8/14
9am	Hoffman II 9am - 9:50am	Brison I 9am - 9:50am	Brison II 9am - 9:50am	Brison III 9am - 9:50am	Littlewood III 9am - 9:50am		
10am	Kaminski II 9:50am - 10:40am	Agterberg II 9:50am - 10:40am	Agterberg III 9:50am - 10:40am	Littlewood II 9:50am - 10:40am	Lesueur II 9:50am - 10:40am		
11am	Coffee 10:40am - 11:10am	Coffee 10:40am - 11:10am	Coffee 10:40am - 11:10am	Coffee 10:40am - 11:10am	Coffee 10:40am - 11:10am		
	Biermann 11:10am - 12:10pm	Brouet 11:10am - 12:10pm	Littlewood I 11:10am - 12pm	Kee 11:10am - 12:10pm	Khomskii 11:10am - 12:10pm		
12pm	Lunch 12:10pm - 1:45pm	Lunch 12:10pm - 1:45pm	Lunch 12pm - 1:45pm	Lunch 12:10pm - 1:45pm	Lunch 12:10pm - 1:45pm		
1pm							
2pm	Agterberg I 1:45pm - 2:35pm	Alloul 1:45pm - 2:45pm		Demsar 1:45pm - 2:45pm	100 years of superconductivity: round table 1:45pm - 4pm		
3pm	3 contrib talks 2:35pm - 3:35pm	Special topic 2:45pm - 3:35pm		3 contributed talks 2:45pm - 3:45pm			
4pm	Break 3:35pm - 6pm	Poster ads 3:35pm - 4:30pm		Break 3:45pm - 6pm			
5pm		Poster session 4:30pm - 7pm					
6pm	Valenti 6pm - 7pm			Lesueur I 6pm - 6:50pm			
7pm	Wiki 7pm - 8pm	Banquet 7pm - 9:30pm		Wiki 6:50pm - 7:50pm			
8pm							
9pm							

ABSTRACTS

MULTIORB 2011 - Talks List

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A2	Alloul	Henri	NMR study of the pressure induced Mott transition to Superconductivity in the newly discovered Cs_3C_{60} isomeric compounds
A3	Bascones	Leni	Iron pnictides as multiorbital antiferromagnets
A4	Basov	Dimitri	Shedding infrared light on high-Tc superconductivity
A5	Batista	Cristian	Lecture 1: Orbital Effects in Frustrated Mott Insulators
	Batista	Cristian	Lecture 2: Lattice of frustrated Molecules
A6	Bierman	Silke	"Effective orbital degeneracy" (and reduction thereof) in correlated systems
A7	Blumberg	Girsh	Raman Spectroscopy of Multiband Superconductors
A8	Brisson	Jean-Pascal	Multigap superconductivity
A9	Brouet	Véronique	New types of electronic orderings in layered cobaltates
A10	Demsar	Jure	Femtosecond time-resolved spectroscopic techniques and their applications to study multi-component order parameter dynamics
A11	Deveraux	Thomas	Introduction to the theory of Fe-based Superconductors
A12	Hoffman	Jennifer	Lecture 1: STM determination of pairing symmetry in cuprates and pnictides
	Hoffman	Jennifer	Lecture 2: STM evidence for orbital ordering in cuprates and pnictides
A13	Kaminski	Adam	Angle Resolved Photoemission Spectroscopy as a probe of unconventional superconductors
A14	Kee	Hae-Young	Unveiling a nematic quantum critical point in multi-orbital systems
A15	Khomskii	Daniel	Charge transfer systems and oxygen holes
A16	Lesueur	Jérôme	Two dimensional electron gas physics at $SrTiO_3$ interfaces
A17	Littlewood	Peter	Condensation of excitons and polaritons
A18	Paglione	Johnpierre	Introduction to iron-based superconductors: interplay of structural, magnetic and superconducting states
A19	Perkins	Natasha	Quasi one-dimensional magnetism in vanadium oxides with orbital degeneracy
A20	Rullier-Albenque	Florence	Multiband description of the transport properties in the iron pnictides
A21	Schmalian	Jörg	Lecture 1: Graphene: introduction and the role of the Coulomb interaction
	Schmalian	Jörg	Lecture 2: Quantum critical scaling in graphene
	Schmalian	Jörg	Lecture 3: Hydrodynamic transport in graphene and ultra-fast dynamics in graphene
A22	Valenti	Roser	Frustration and multiorbital effect in Mott insulators and superconductors: an ab initio point of view
A23	Van den Brink	Jörg	Orbital degrees of freedom in strongly correlated transition metal compounds
A24	Vojta	Matthias	Lecture 1: Mott transitions - an introduction
	Vojta	Matthias	Lecture 2: Orbital-selective Mott transitions: Concepts
	Vojta	Matthias	Lecture 3: Orbital-selective Mott transitions: Examples
A25	Zhang	Shoucheng	Topological insulators and superconductors

Daniel Agterberg

Department of Physics University of Wisconsin – Milwaukee, USA

Superconductivity without Parity Symmetry

These lectures will provide a pedagogical overview of superconductors in materials that do not have a center of inversion symmetry. Two key symmetries underlie the formation of superconductivity: parity (inversion) and time reversal. The role of breaking parity symmetry is much less well understood than the role breaking time reversal symmetry on superconductivity. However, this has become an important issue since many materials lack inversion symmetry. Two recent relevant examples are the metallic interface between SrTiO_3 and LaAlO_3 (where superconductivity has been discovered), and the surface of topological insulators. In these lectures, I will discuss: microscopic theories of superconductors without inversion symmetry (including a generalized Rashba spin-orbit interaction which plays an essential role); phenomenological theories and related magnetoelectric effects; and new physics that arises in magnetic fields (including “universal” spin susceptibility, helical phases, fractional vortices, and Majorana modes).

Henri Alloul

Laboratoire de Physique des Solides, UMR 8502 CNRS, Université Paris-Sud 91405, Orsay (France)

NMR study of the pressure induced Mott transition to Superconductivity in the newly discovered Cs₃C₆₀ isomeric compounds

The discovery in 1991 of high temperature superconductivity in A₃C₆₀ compounds, where A is an alkali ion, has been rapidly ascribed to a BCS mechanism, in which the SC pairing is mediated by on ball optical phonon modes. While this has lead to consider that electronic correlations were not important in these compounds, further detailed studies of various A_nC₆₀ compounds with $n = 1, 2, 4$ [1-3] allowed to evidence that the electronic properties of these compounds cannot be explained by a simple progressive band filling of the C₆₀ six-fold degenerate t_{1u} molecular level. This could only be ascribed to the influence of electron correlations and of Jahn-Teller Distortions (JTD) of the C₆₀ ball, which energetically favour evenly charged C₆₀ molecules [1].

We shall report the recent discovery of two expanded fulleride Cs₃C₆₀ isomeric phases which are Mott insulators at ambient pressure [4-5]. Both phases undergo a pressure induced first order Mott transition to superconductivity with a (ρ , T) phase diagram displaying a dome shaped superconductivity, a common situation encountered nowadays in correlated electron systems [5].

NMR experiments allowed us to study the magnetic properties of the Mott phases which exhibit a low spin $S=1/2$ state. We do evidence the onset of enhanced spin fluctuations with decreasing pressure towards the Mott transition, and could follow the phase diagram up to a critical point near room T , analogous to that observed at the liquid-gas transition.

So, although superconductivity admittedly results from an electron-phonon mechanism, the incidence of electron correlations has an importance on the electronic properties, as had been anticipated from DMFT calculations [6]. These results establish then the existence of a clear Mott transition to a superconducting state in 3D systems in which the multi-orbital molecular state degeneracy has been lifted by JTD.

- [1] M. Capone,, M. Fabrizio, P. Giannozzi and E. Tosatti, Phys. Rev. B **62**, 7619 (2000).
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Elena (Leni) Bascones

Instituto de Ciencia de Materiales de Madrid (ICMM-CSIC), Madrid, Spain

Iron pnictides as multiorbital antiferromagnets

A major breakthrough took place in 2008 with the discovery of high temperature superconductivity in iron pnictides. The basic structure of these materials are FeAs layers. Superconductivity has been also found in iron chalcogenides with related FeSe/FeTe layers. In these materials superconductivity emerges when doping or applying pressure to an antiferromagnetic compound. Most iron pnictides order with $(\pi,0)$ momentum, antiferromagnetic in the x direction and ferromagnetic in the y direction. Double stripe and more complex structures have been found in iron chalcogenides. The magnetic state of iron pnictides is metallic and presents unusual magnetic moment and resistivity anisotropy [1].

The origin of magnetism in iron superconductors is still unsettled. At the heart of the debate it is the itinerant (weak coupling) versus localized (strong coupling) nature of magnetism. The itinerant picture relies on the metallicity of the magnetic state and an approximate $(\pi,0)$ nesting of the Fermi surface. In the strong coupling picture localized moments interact with AF exchange constants J_1 and J_2 with their first and second nearest neighbors respectively. $(\pi,0)$ state can be stabilized with $J_1 < 2 J_2$, but little is known on the actual value of these constants. Both the itinerant and localized models are minimal descriptions which can be derived from more elaborate microscopic descriptions. Iron pnictides are multiorbital systems and such a microscopic description has to include all the orbitals relevant to magnetism.

In the talk I will discuss magnetism in iron pnictides starting from a five-orbital model [2]. We will approach the magnetic state from both strong coupling (Heisenberg) and weak coupling (Hartree-Fock) perspective. I will discuss the value of the exchange constants J_1 and J_2 and their dependence on the Hund's coupling [3]. We will see the magnetic phases which appear in each picture, including a low magnetic phase which violates Hund's rule and that can be understood in terms of orbital dependent exchange constants [4]. Orbital ordering will be seen to appear naturally in the $(\pi,0)$ state.

If time allows if I will discuss on the role played by orbital ordering on the appearance of resistivity anisotropy in the magnetic state[5].

[1] For a review see, J. Paglione and R.L. Greene, Nature Phys. **6**, 645 (2010).

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Dmitri N. Basov

University of California San Diego, USA - <http://infrared.ucsd.edu/>

Shedding infrared light on high-Tc superconductivity

The mechanism of high-Tc superconductivity is one of the most challenging unresolved problems in contemporary physics. The discovery of high Tc superconductivity in the iron pnictides, while interesting in itself, offers a new perspective on several aspects of cuprate high-Tc superconductors. My plan is to overview common patterns as well as contrasting trends between the two classes of high-Tc materials, focusing on the information generated through infrared/optical probes. Infrared methods enable experimental access to the superconducting energy gap and pseudogap, strong coupling effects responsible for pairing, the collective response of the superfluid and allow one to quantify the strength of electronic correlations [Nature-Physics **5**, 647 (2009), Reviews of Modern Physics **83**, 471 (2011)]. With this panoramic view of effects central for our understanding of superconductivity I will attempt to identify factors favoring higher Tc in exotic superconductors [Nature-Physics **7**, 271 (2011)].

Cristian Batista

Los Alamos National Laboratory, USA

Lecture 1: Orbital Effects in Frustrated Mott Insulators

In the first lecture I will derive the effective charge and current density operators for a single-band Hubbard model in the strong coupling limit. We will see that frustration is prerequisite for obtaining nontrivial expressions of these effective operators, and consequently, for observing inhomogeneous charge and current distributions in Mott insulators. In particular, we will identify the types of magnetic orderings that lead to charge-density-waves and the ones that produce a distribution of orbital currents. By the end of the lecture, I will discuss the algebraic structure of the current and charge density operators and derive a few consequences for the dynamical response of frustrated Mott insulators.

Lecture 2: Lattice of frustrated Molecules

In the second lecture I will show how multi-orbital physics emerges from single-orbital Hubbard models defined on lattices of frustrated molecules. In particular, I will derive interesting magneto-electric effects that arise in these lattices and may be relevant for some families of organic Mott insulators. These examples will illustrate in a pedagogic way how frustration can lead to a useful and interesting interplay between spin and charge degrees of freedom in frustrated Mott insulators.

Silke Biermann,

CPHT Ecole Polytechnique, France

**``Effective orbital degeneracy" (and reduction thereof)
in correlated systems**

We will discuss the Mott transition in multi-orbital Hubbard models, with particular emphasis on the interplay of crystal field splitting and correlation effects.

On the specific examples of V_2O_3 and $YTiO_3$ we will introduce the concept of a reduced effective orbital degeneracy, leading to orbital-selective coherence in V_2O_3 , and orbital order in $YTiO_3$.

In the second part, we will show how spin-orbit interactions can have similar effects, leading e.g. to Mott insulating behavior in Sr_2IrO_4 and spin-orbital polarization in Sr_2RhO_4 .

Finally, we will comment on theoretical tools for describing this kind of interplay of correlations, crystal-fields, and spin-orbit interactions from first principles.

Girsh Blumberg

Rutgers, The State University of New Jersey

Raman Spectroscopy of Multiband Superconductors

High-resolution electronic Raman scattering has become an indispensable tool in the study of magnetic and electronic excitations in novel superconductors. One of the most illustrious achievements of polarized electronic Raman scattering has been the ability to focus on the nature of electron dynamics in different regions of the Brillouin zone in which charge excitations can be selectively mapped and analyzed using group-theoretical symmetry arguments. This distinguishes Raman scattering from most other transport and thermodynamic measurements, allowing for the study of the development of correlations in projected regions of the Brillouin zone.

Electronic Raman scattering has played a major role in characterizing the anisotropic dynamics of electrons across the phase diagram of cuprate superconductors. This includes the study of antiferromagnetism, where Raman measurements on the parent insulating cuprate compounds yielded an estimate of the magnetic exchange interaction strength from the energy of the two-magnon scattering. Raman spectroscopy has provided new insights into unconventional superconductivity, including the symmetries of the superconducting order parameters, the nature and properties of the in-gap collective modes, and clear signatures of the multi-band effects.

We will review results of electronic and magnetic Raman spectroscopic studies from several families of superconductors and related compounds: (1) by analyzing two-magnon Raman scattering for parent and lightly doped superconducting compounds we establish the evolution of magnetically ordered state; from the interpretation of two-magnon scattering bands we make a quantitative estimate of the exchange interaction strength; (2) from systematic phononic, magnetic and electronic polarized Raman scattering data as a function of temperature we evaluate an interplay between structural, magnetic, and superconducting transitions; (3) using polarized ultra-low-frequency electronic Raman scattering data we examine the symmetry of the superconducting order parameter, the magnitude of the superconducting gaps and their evolution.

Jean-Pascal Brison

SPSMS, UMR-E CEA/UJF Grenoble 1, INAC, Grenoble, France

Multigap superconductivity

Lecture 1: We will review rapidly some historical aspects on multigap superconductivity, to precise what it is and where it may originate from. Time will be spent on the paradigm of multigap superconductivity, MgB₂, which gave the first unquestionable example of such a superconductor, allowing for experimental and theoretical exploration of the phenomena.

Lecture 2: We will review various experimental probes and manifestations of multigap superconductivity, relying mainly on the example of MgB₂. In particular, we will discuss microscopic and macroscopic probes of multigap behaviour, and how they can (or not) distinguish multigap, and unconventional superconductivity .

Lecture 3: We will discuss examples of multigap superconductors, both on “well established cases” and on systems where it is believed that such a phenomenon should happen. Important families of such superconductors include the dichalcogenides, the iron pnictides, heavy fermion superconductors, non centrosymmetric systems as well as ferromagnetic superconductors.

Véronique Brouet

Laboratoire de Physique des Solides, CNRS-Université Paris-Sud, France

New types of electronic orderings in layered cobaltates

The study of layered cobaltates, a family where triangular planes of Co (with formula CoO_2) host a tunable number of electrons, developed after the discovery in 2003 of superconductivity at 4K in one of their phases [1]. It was believed that this compound could be described as doped Mott insulators, possibly sharing important characteristics with the superconducting cuprates. In the following, it was realized that the phase diagram is rather complicated [2,3] and that, surprisingly, sign of strong correlations in the metallic phases (namely high effective masses, non-Pauli susceptibilities or high thermoelectric powers) seem to appear - and in fact increase - far from the Mott insulator, near the band insulator limit. In the same doping region, NMR showed that the Co sites are not all equivalent, but that some sites have trapped an electron [4]. This charge order within a metallic phase is rather unusual and may be linked to the structure of the planes intercalated between the CoO_2 planes. Many studies aim at understanding whether this peculiar charge order is the source of the consequence of the unusual correlations found in these families [3].

In this lecture, I will first review the main properties of these families and then focus on how Angle Resolved Photoemission experiments [5,6] can help to understand the electronic structure of these materials, especially the role of the different orbitals, the nature of the correlations and the impact of charge orders.

[1] R.E. Schaak et al., *Nature* **424**, 527 (2003)

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[5] D. Qian et al., *PRL* **97**, 186405 (2006) ; H.B. Yang et al., *PRL* **95**, 146401 (2005)

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Jure Demsar

Physics Department, University of Konstanz, D-78457, Germany

Femtosecond time-resolved spectroscopic techniques and their applications to study multi-component order parameter dynamics

In recent years we are experiencing a major progress in the development of femtosecond ($1 \text{ fs} = 10^{-15} \text{ s}$) time resolved spectroscopic techniques and their applications to studying dynamics of correlated electron systems. These techniques enable studies of the dynamics of complex dielectric function over broad spectral range from 0.1 terahertz ($1 \text{ THz} = 4.1 \text{ meV} = 33 \text{ cm}^{-1}$) to several eV, the dynamics of changes in the electron distribution and the electronic band structure using time and angular resolved photoemission (tr-ARPES), as well as studies of the underlying structural dynamics using femtosecond time-resolved X-ray diffraction of femtosecond electron diffraction. Such experiments can be performed in the weak perturbation regime, where the system under investigation is close to its thermodynamic equilibrium, or in the high excitation regime, where phase transitions between different thermodynamic states can be studied with femtosecond time resolution.

After review of the existing femtosecond time-resolved techniques I will present several examples of such studies, focusing on superconductors studied with time-resolved THz techniques. I will first present results of studies on conventional BCS low- T_c superconductor NbN, following with results on cuprate superconductors and summarize the first results on multi-gap pnictide high temperature superconductors.

Thomas Peter Devereaux

SLAC National Accelerator Laboratory, Stanford University, Stanford CA, USA

Introduction to the theory of Fe-based Superconductors

The quantum chemistry of Fe: understanding the basics of the pnictides. Atomic chemistry of Fe in different materials. Unit cells, band structures and band characters. Correlated electrons in solids. How is Fe different than Cu? Effective Hamiltonians.

Ordered phase in the pnictides. Landau quasiparticle concepts. Charge and spin density waves. BCS theory of superconductivity and pairing from attractive interactions; unconventional pairing from repulsive interactions. Weak and strong coupling scenarios for magnetism and superconductivity. Role of orbital degrees of freedom; phonons.

Using photon spectroscopies to explore bandstructures, correlations, and pairing. Quick introductions to angle-resolved photoemission, x-ray absorption, and Raman spectroscopy in the pnictides.

Jennifer Hoffman

Department of Physics, Harvard States University, USA

STM determination of pairing symmetry in cuprates and pnictides

This lecture will start with an explanation of conventional scanning tunneling microscopy (STM), and how it can be expanded from a real space imaging tool to a simultaneous momentum space imaging tool using quasiparticle interference (QPI). I will then talk about how this tool can be applied towards a phase-sensitive determination of the pairing symmetry in cuprate and pnictide superconductors. In particular, in the pnictide superconductors, up to five Fe *d* bands cross the Fermi level, which allows many possibilities for pairing symmetry. Because of the momentum space configurations of these bands, the pnictide pairing symmetry is more challenging to extract from bulk transport than it was in cuprates. However, STM can provide clear, phase-sensitive evidence that the superconducting order parameter varies from nodeless to nodal s_{\pm} in the FeTe_{1-x}Se_x system of superconductors.

STM evidence for orbital ordering in cuprates and pnictides

The route to a theoretical understanding of high-T_c superconductivity must likely include a characterization of the 'normal' state out of which superconductivity arises. In cuprates, this means identifying the mysterious 'pseudogap' phase in which Fermi level density of states is suppressed before bulk superconductivity is established. In pnictides, this means understanding the possibly coupled nematic, structural, and magnetic transitions which precede the superconducting transition on the underdoped side. As a step towards achieving these goals, I will explain how the effective spatial resolution of STM can be enhanced using Fourier-based algorithms, to allow visualization of the sub-unit-cell distribution of states. In both cuprates and pnictides, recent high-resolution STM studies have shown evidence for orbital ordering as a possible origin of the pseudogap, and possible explanation of anisotropic transport properties in pnictides.

Adam Kaminski

Associate Professor and Associate Scientist Ames Laboratory and Department of Physics and Astronomy Iowa State University

Angle Resolved Photoemission Spectroscopy as a probe of unconventional superconductors

Over last decade or so, ARPES experienced rapid evolution thanks to new synchrotron light sources, introduction of modern electron analyzers and improvements in single crystal growth. More than order of magnitude improvement in energy/momentum resolution and data acquisition rate moved this technique from an art form to routine tool in condensed matter physics. In the course of those lectures I will present an overview of basic principles of this technique along with the physical properties it can explore. I will also provide rich set of examples how it improved our understanding of physics of various systems with special focus on multiorbital superconductors.

Hae-Young Kee,

University of Toronto, Canada

Unveiling a nematic quantum critical point in multi-orbital systems

A variety of transition metal materials such as Ru-oxides and Fe-pnictides, has been proposed to harbour an electronic nematic phase. In particular, $\text{Sr}_3\text{Ru}_2\text{O}_7$ is a promising candidate for nematicity as it exhibits a magneto-resistive in-plane anisotropy within a finite magnetic field window bounded by meta-magnetic transitions. This is consistent with earlier theoretical studies showing that the isotropic-nematic transition is generically first order and is accompanied by a meta-magnetic jump when tuned by a magnetic field.

Interestingly, $\text{Sr}_3\text{Ru}_2\text{O}_7$ was initially considered to be a prototype for the study of quantum critical phenomena, exhibiting a pronounced non-Fermi liquid resistivity. In addition to non-Fermi liquid transport, specific heat also shows critical behaviour, suggesting the existence of an unidentified quantum critical point related to the nematic phase. In this talk, I will first review the concept of electronic nematic phase, recent theoretical developments, and its experimental consequences. I will then show that orbital degrees of freedom play an essential role in revealing a hidden nematic quantum critical point, even though it is overshadowed by a nearby meta-magnetic transition at low temperature. I will further discuss our findings in light of the phenomena observed in multi-orbital materials.

Daniel Khomskii

Pr. Dr. - II Physikalisches Institut, Universitaet zu Koeln, Germany

Charge transfer systems and oxygen holes

Often, considering correlated systems, one pays the main attention to the d-electrons themselves - to their correlations, orbital character, magnetic properties etc. However in real materials usually also the p-electrons of ligands, e.g. oxygens, play an important role. Especially important their role becomes in case of small or negative charge transfer gap, in which case there exist a lot of oxygen holes. In my lecture I will describe this situation and discuss some specific effects observed in this regime, such as the self-doping and the appearance of ferromagnetism, spontaneous charge disproportionation, etc. Possible relevance of ligand holes for superconductivity of such systems will be also discussed.

Jérôme Lesueur – Nicolas Bergeal

Laboratoire de Physique et d'Etude des Matériaux ESPCI - UPMC – CNRS, Paris France

Two dimensional electron gas physics at SrTiO₃ interfaces

In the recent years, highly controlled growth of oxides layers has been achieved, leading to almost defect free epitaxial interfaces. Hallmarks are perovskite based structures on SrTiO₃. The electronic reconstruction that takes place at the interface gives rise to a two dimensional electron gas (2DEG) of very high mobility, which has been studied experimentally. The subtle orbital arrangements at the interface, combined with the quantum paraelectric behavior of SrTiO₃ lead to a very rich phase diagram where electronic orders may appear (superconductivity, magnetism, orbital orders ...), strong correlations play a role, and strong confinement effects as well, like Rashba spin-orbit coupling for example. By modulating the carrier density of the 2DEG with a gate voltage, one can go all over this very fascinating physical landscape with a powerful control knob. Such interfaces have also tremendous potentialities in terms of applications.

In this lecture we will present :

- the bulk properties of SrTiO₃
- the growth and structural properties of SrTiO₃ based heterostructures
- the electronic surface reconstruction in these heterostructures
- their electronic properties (mostly LaAlO₃/SrTiO₃ and LaTiO₃/SrTiO₃)

and then focus on the LaTiO₃/SrTiO₃ system :

- superconductivity at a band insulator/Mott insulator interface
- the electronic phase diagram
- magneto-transport, localization and Rashba coupling

Condensation of excitons and polaritons

Peter Littlewood

*Argonne National Laboratory, Argonne IL
James Franck Institute, University of Chicago
Cavendish Laboratory, University of Cambridge*

Macroscopic phase coherence is one of the most remarkable manifestations of quantum mechanics, yet it seems to be the inevitable ground state of interacting many-body systems. In the last two decades, the familiar examples of superfluid He and conventional superconductors have been joined by exotic and high temperature superconductors, ultra-cold atomic gases, both bosonic and fermionic, and recently systems of excitons, magnons, and exciton-photon superpositions called polaritons, the subject of this talk.

An exciton is the solid-state analogue of positronium, made up of an electron and a hole in a semiconductor, bound together by the Coulomb interaction. The idea that a dense system of electrons and holes would be unstable toward an excitonic (electrical) insulator is one of the key ideas underlying metal-insulator transition physics. The further possibility that an exciton fluid would be a Bose-Einstein condensate was raised over 40 years ago, and has been the subject of an extensive experimental search in a variety of condensed matter systems. Such a condensate would naturally exhibit phase coherence. Lately, some novel experiments with planar optical microcavities make use of the mixing of excitons with photons to create a composite boson called a polariton that has a very light mass, and is thus a good candidate for a high-temperature Bose condensate. Good evidence for spontaneous coherence has now been obtained, though there are special issues to resolve considering the effects of low dimensionality, disorder, strong interactions, and especially strong decoherence associated with decay of the condensate into environmental photons --- since the condensate is a special kind of laser.

These lectures will address: exciton formation in semiconductors, the predicted coherent ground state, and the BCS to BEC crossover; unbalanced electron-hole systems and analogies to FFLO; coupling to photons in microcavities and the formation of polaritons as a composite boson; polariton BEC; open system dynamics and decoherence; driven polaritons and quantum dynamics.

Johnpierre Paglione

*Assistant Professor Center for Nanophysics and Advanced Materials Department of Physics,
University of Maryland, USA*

Introduction to iron-based superconductors: interplay of structural, magnetic and superconducting states

The discovery of high-temperature superconductivity in iron-based compounds has sparked a flurry of activity in the condensed matter physics community. With transition temperatures reaching close to 60 K, this exciting and rapidly expanding field of research has caused a surge of experimental and theoretical activity devoted to understanding this new family of materials. I will provide an overview of important research efforts in growth and characterization of iron-pnictide compounds, as well as key experimental observations contributing to our current understanding of the nature of superconductivity in this family of compounds, focusing on phase diagrams and superconducting gap symmetry. In addition, I will present a summary of our recent efforts in addressing the relation between superconductivity, magnetism and crystallographic structure. The importance of internal tetrahedral structure in stabilizing both magnetic and superconducting ground states is addressed through an investigation of solid solutions of (Ba,Sr,Ca)Fe₂As₂ series of parent compounds. In addition, by inducing the "collapsed" form of the tetragonal unit cell of the 122 series via rare earth substitution in (Ca,R)Fe₂As₂, we investigate the role of indirect electron doping on the evolution of ground states while controlling the interlayer pnictogen-pnictogen bonding via chemical pressure.

Reference:

J. Paglione and R.L. Greene, *Nature Physics* **6**, 645 (2010).

Natalia Perkins

Assistant Professor, Department of Physics, University of Wisconsin-Madison, USA

Quasi one-dimensional magnetism in vanadium oxides with orbital degeneracy

Geometrically frustrated magnets with orbital degeneracy exhibit a variety of complex ground states with unusual magnetic and orbital orders. In my talk, I will focus on vanadium oxides with general formula AV_2O_4 in which orbital fluctuations strongly influence magnetic properties and give rise to novel properties not observed in purely spin materials. I will discuss two vanadium compounds: a spinel ZnV_2O_4 and a quasi-one-dimensional compound CaV_2O_4 . The vanadium chains in these compounds are characterized by frustrated magnetic interactions, Ising-like orbital exchanges and a relativistic spin-orbit interaction.

On these two examples I will show how the interplay between spin, orbital and lattice degrees of freedom leads to a variety of interesting ground states and elementary excitations.

Florence Rullier-Albenque

Service de Physique de l'Etat Condensé. Orme des Merisiers, IRAMIS, CEA-Saclay (CNRS URA 2464), F-91191 Gif sur Yvette Cedex, France

Multiband description of the transport properties in the iron pnictides

The electronic structure of the iron-based superconductors is characterized by the presence of both hole and electron bands at the Fermi level. It was found that the size of these pockets can be changed by different types of substitution. These multiband effects have important consequences on the evolution of the transport properties, as doping induces imbalance between holes and electrons.

In this talk, I will review the evolution of the transport properties with doping in the 122 family BaFe_2As_2 , for which sizeable single crystals required for transport measurements are available. The combined resistivity and Hall effect measurements will be analyzed using a minimal two-band model more specifically in the case of the electron doped BaFe_2As_2 using Co [1] or Ni [2] and for the isovalent Ru substituted BaFe_2As_2 compound [3], in association with ARPES measurements performed on the same samples [4,5]. Recent magnetoresistance data in the paramagnetic phase of these compounds will be also discussed.

[1] F. Rullier-Albenque, D. Colson, A. Forget and H. Alloul, *Phys. Rev. Lett.* **103**, 057001 (2009).

[2] A. Olariu, F. Rullier-Albenque, D. Colson and A. Forget, *Phys. Rev. B* **83**, 054518 (2011).

[3] F. Rullier-Albenque, D. Colson, A. Forget, P. Thuéry and S. Poissonnet, *Phys. Rev. B* **81**, 224503 (2010).

[4] V. Brouet et al., *Phys. Rev. B* **80**, 165115 (2009).

[5] V. Brouet, F. Rullier-Albenque, M. Marsi et al., *Phys. Rev. Lett.* **105**, 087001 (2010).

Jörg Schmalian

Professor für Physik Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie Karlsruhe, Germany

1. Graphene: introduction and the role of the Coulomb interaction

We will give a brief introduction into the physical properties of graphene along with a tight binding description of the states near the Fermi energy and the linear Dirac spectrum near the Fermi points. Next we will discuss the role of the electron-electron Coulomb interaction on graphene and contrast the behavior to what is found in the usual non-relativistic electron gas. We also discuss the role of the substrate and potential screening of the Coulomb interaction by nearby metallic plates.

2. Quantum critical scaling in graphene

We discuss the notion of scaling near critical points and establish the fact that graphene at the neutrality point behaves as a system at a critical point. Using a renormalization group calculation and scaling arguments we derive the low temperature, low density etc. behavior of various thermodynamic and transport quantities.

3. Hydrodynamic transport in graphene and ultra-fast dynamics in graphene

We use the previously established scaling description of graphene to analyze the temperature dependence of the d.c. susceptibility of clean graphene. Here we will encounter some interesting pseudo-conservation law of holes and electrons under leading order Coulomb interaction which enables us to make sharp predictions for the T-dependence of the d.c. conductivity and viscosity. This allows to make statements about the perfect fluid behavior of graphene and the possibility of electron turbulence. We finally demonstrate implications of the mentioned pseudo-conservation law for the ultra-fast dynamics of graphene.

Roser Valenti

Institute of Theoretical Physics, Goethe University Frankfurt, Germany

Frustration and multiorbital effects in Mott insulators and superconductors: an ab initio point of view

In this talk, we shall present an introductory overview of multiorbital physics and frustration effects in some families of Mott insulators (spinel, pyrochlores) and superconductors (iron pnictides) by considering a combination of ab initio density functional theory and effective model considerations.

Jeroen Van Den Brink

IFW Dresden, Institute for Theoretical Solid State Physics, Dresden, Germany

Orbital degrees of freedom in strongly correlated transition metal compounds

- Introduction to open d-shell systems, spin and orbital degrees of freedom, strong electronic correlations, Hubbard U and Hund J.
- Local orbital splittings due to crystal fields and Jahn-Teller effect.
- Cooperative orbital physics: cooperative Jahn-Teller, spin-orbital interactions, orbital-orbital interactions, Kugel-Khomskii Hamiltonians and how they can be derived from multi-orbital Hubbard models.
- Goodenough-Kanamori-Anderson rules for superexchange, orbital order and spin-orbital order, orbital excitations and orbitons.
- Examples of orbital ordering in real materials.
- Double- and superexchange, their competition and examples of resulting groundstates in manganites.
- Compass models: orbital-only compass models, 90 and 120 degree compass models.
- Kitaev's honeycomb model, intermediate symmetries between local (gauge) and global, nematic ordering, order by disorder in compass models.
- Relation to iridates and 5d materials with strong relativistic spin-orbit coupling.

Optional extra topics:

1. Measuring spin and orbital excitations with resonant inelastic x-ray scattering.
2. Multiferroicity, in particular in multi-orbital materials.

Matthias Vojta

Pr. Dr., Institut fuer Theoretische Physik, Technische Universitaet, Dresden, Germany

- 1. Mott transitions - an introduction**
- 2. Orbital-selective Mott transitions: Concepts**
- 3. Orbital-selective Mott transitions: Examples**

Non-Fermi liquid behavior is observed experimentally in a variety of strongly correlated electron materials, but remains poorly understood. Among the interesting theoretical concepts is that of an orbital-selective Mott phase, where conduction electrons undergo a partial Mott localization. This concept is intimately related to the breakdown of the Kondo effect in heavy-fermion metals, and to the occurrence of metallic spin-liquid phases.

In these lectures, I will start by reviewing our current understanding of Mott transitions. Then I will introduce basic ideas and available theories for orbital-selective Mott behavior and construct a "global" phase diagram. Finally, I will discuss proposals for its experimental realization in heavy-fermion compounds, iron-pnictide superconductors, and cuprates.

Xiao-Liang Qi^{1,2} and Shou-Cheng Zhang²

1. Microsoft Research, University of California, Santa Barbara, CA 93106, USA

2. Department of Physics, Stanford University, Stanford, CA 94305

Topological insulators and superconductors

Topological insulators are new states of quantum matter which cannot be adiabatically connected to conventional insulators and semiconductors. They are characterized by a full insulating gap in the bulk and gapless edge or surface states which are protected by time-reversal symmetry. These topological materials have been theoretically predicted and experimentally observed in a variety of systems, including HgTe quantum wells, BiSb alloys, and Bi₂Te₃ and Bi₂Se₃ crystals. We review theoretical models, materials properties and experimental results on two-dimensional and three-dimensional topological insulators, and discuss both the topological band theory and the topological field theory. Topological superconductors have a full pairing gap in the bulk and gapless surface states consisting of Majorana fermions. We review the theory of topological superconductors in close analogy to the theory of topological insulators.

arXiv:1008.2026, to be published in RMP Sept 2011

POSTERS SESSIONS

MULTIORB 2011 - ABSTRACTS AND POSTERS SESSIONS

N°	Family Name	First Name	Title
P1	Brouet	Véronique	Comparison of Fermi Surface and Band Structure measured with ARPES in $\text{Ba}(\text{Fe}_{0.65}\text{Ru}_{0.35})_2\text{As}_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$
P2	Das	Tanmoy	Double spin resonances in pnictide due to the effects of multiband and multiple superconducting gaps
P3	Deng	Xiaoyu	Strong correlations in LaNiO_3 and electronic origin of photonem
P4	Fanfarillo	Laura	Theory of fluctuations in multiband superconductor: Application to pnictides
P5	Fisher	Mark Hannes	Mean-Field Analysis of Intra-Unit-Cell Order in the Emery Model
P6	Golosov	Denis	New correlated model of colossal magnetoresistive manganese oxides
P7	Gonzalez Quintela	Camilo	Electronic, magnetic and structural properties of $\text{Cr}_{1-x}\text{V}_x\text{N}$
P8	Gukelberger	Jan	Diagrammatic Monte Carlo for the Hubbard model
P9	Hajlaoui	Madhi	Electron spectroscopy on Strongly Correlated systems
P10	Hoek/Coneri	Marcel/Frances	At the interface between P- and N-type doped Mott insulators
P11	Isaev	Leonid	Electronic mechanism for ferroelectricity and strong magneto-electric coupling in charge-ordered multiferroics
P12	Jia	Chunjing	Numerical study of momentum dependent resonant inelastic x-ray scattering (RIXS) of cuprates
P13	Kato	Yasuyuki	Orbital disorder induced by charge fluctuations in vanadium spinels
P14	Kemper	Alexander	Effects of multiple orbitals on spin-fluctuations in the ferro-pnictides
P15	Knolle	Johannes	Multiorbital spin susceptibility in a magnetically ordered state - Orbital versus excitonic spin density wave scenario

MULTIORB 2011 - ABSTRACTS AND POSTERS SESSIONS

N°	Family Name	First Name	Title
P16	Krannich	Sven	Lattice and spin dynamics of FeSi by inelastic neutron spectroscopy
P17	Kung	Yvonne	Charge and spin order in the time domain for transition metal correlated systems
P18	Lin	Ping-Hui	Electronic structure of Iron-Chalcogenide Superconductors observed by Angle Resolved Photoemission Spectroscopy
P19	Maiti	Saurabh	Relating $2\Delta/T_c$ on hole Fermi surface to nodes in Iron based Superconductors
P20	Marra	Pasquale	Spin and orbital excitations probed with resonant inelastic X-Ray scattering
P21	Martins	Cyril	Interplay of Spin-Orbit Coupling and Electronic Coulomb Interactions in strontium iridate (Sr ₂ IrO ₄)
P22	Mazo	Victoria	Quantum hall edge states in bilayer graphene ribbons
P23	Michal	Vincent	Field-Induced Spin-Exciton Condensation in dx ² -y ² -wave Superconductivity
P24	Mravlje	Jernej	Why in Sr ₂ RuO ₄ electrons in the widest band have largest mass?
P25	Nicolaou	Alessandro	Novel electronic states in misfit cobaltates investigated by ARPES
P26	Ong	Tze Tzen	Fe Impurity in As Tetrahedron
P27	Putzke	Carsten	Fermi-surface study of the iron pnictide superconductors LiFeP and LiFeAs
P28	Ramires Neves de Oliveira	Aline	Theory for electron spin resonance in YbAlB ₄
P29	Taleb	Amina	Angle Resolved Photoelectron Spectroscopy and Applications
P30	Taupin	Mathieu	Thermal conductivity in the ferromagnetic superconductor UCoGe

MULTIORB 2011 - ABSTRACTS AND POSTERS SESSIONS

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P31	Texier	Yoan	NMR study of magnetism and superconductivity in pnictides
P32	Trousselet	Fabien	Magnetism in the Kitaev-Heisenberg model with spin vacancies
P33	Um	Youngje	Raman light scattering on the $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Se}_x$ and LiFeAs
P34	Wang	Yan	Volovik effect in a highly anisotropic multiband superconductor: experiment and theory
P35	Wang	Wenya	Coexistence of spin density waves (SDW) and superconductivity (SC) in electron-doped cuprates
P36	Winograd	Emilio Andres	Orbital selective crossovers and symmetry restoration in an asymmetric Hubbard model of cold atoms in optical lattices
P37	Yusufaly	Tahir	Harnessing competition in ferroelectric superlattices to engineer enhanced piezoelectrics

Comparison of Fermi Surface and Band Structure measured with ARPES in $\text{Ba}(\text{Fe}_{0.65}\text{Ru}_{0.35})_2\text{As}_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$

Véronique Brouet, M. Marsi, B. Mansart, M.F. Jensen, Y. Texier, Laboratoire de Physique des Solides d'Orsay, UMR8502, France

A. Taleb-Ibrahimi, P. Le Fèvre, F. Bertran, A. Nicolaou, CASSIOPEE beamline, Synchrotron SOLEIL, France

D. Colson, A. Forget, F. Rullier-Albenque, SPEC, CEA Saclay (CNRS URA 2464), France

We present a compared investigation of the electronic structure of two families of iron pnictides, where superconductivity is achieved either by electron doping or by isovalent substitution. We observe that Co substitution leads to an electron doping of the electronic structure, in good agreement with a rigid band filling picture [1]. We also observe that Ru substitution yields a coherent electronic structure, with the same number of holes and electrons, i.e. with no induced doping [2]. However, these two numbers are about twice larger than in BaFe_2As_2 , suggesting the absolute number of carriers is an adjustable parameter of the electronic structure. Simultaneously, we observe a large increase of the Fermi velocities. These observations present interesting analogies with those described in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$. These studies show that superconductivity takes place in quite different environment in doped and undoped superconductors.

[1] V. Brouet *et al.*, Phys. Rev. B **80**, 165115 (2009) and cond-mat/1105.5604

[2] V. Brouet *et al.*, PRL **105**, 087001 (2010)

Double spin resonances in pnictide due to the effects of multiband and multiple superconducting gaps

Tanmoy Das, A. V. Balatsky – Los Alamos National Laboratory, USA

We have shown that for a multiband system with unconventional pairing with sign-changing gaps, one expects to find multiple spin resonances which are separated both in energy and momenta.[1] We calculate the RPA-based spin resonance spectra of pnictide superconductor using five bands tight-binding model or angle-resolved photoemission spectroscopy (ARPES) Fermi surface (FS) and experimental values of superconducting (SC) gaps. The essential mechanism for having two resonances in pnictide is the splitting between two hole pockets with different gap amplitudes. The resonance spectra split both in energy and momenta due to the effects of multiband and multiple gaps in a s_{\pm} -pairing; the higher energy peak appears around the commensurate momenta due to scattering between α -FS to γ/δ -FS pockets. The second resonance is incommensurate coming from β -FS to γ/δ -FS scatterings and its q -vector is doping dependent—hence on the FS topology. Energies of both resonances are strongly doping dependent and is proportional to the gap amplitudes at the contributing FSs. Work is supported by US DOE.

[1] Tanmoy Das and A. V. Balatsky, Phys. Rev. Letts. (2011, in press).

Strong correlations in LaNiO₃ and electronic origin of photonem

Xiaoyu Deng, Michel Ferrero, Jernej Mravlje, Antoine Georges – CPHT Ecole Polytechnique, France

We investigate the electronic structure of LaNiO₃, a charge-transfer metallic oxide with strong electronic correlations. The latter are treated within dynamical mean-field theory combined with density-functional theory. The calculations yield a correlated metal with a mass enhancement over the band value in reasonable agreement with specific heat, thermopower and optical measurements. The kink at ~ -0.25 eV in the quasiparticle dispersion near the δ -point, reported by angular resolved photoemission spectroscopy (ARPES), is accurately reproduced by our calculations. This strongly supports an electronic origin of this feature. Comparison to ARPES raises several open questions, particularly regarding the dispersion of quasiparticles near the M-point and the nature of the t_{2g} electronic states.

Theory of fluctuations in multiband superconductor: Application to pnictides

Laura Fanfarillo, L.Benfatto, S.Caprara, C.Castellani and M.Grilli
'Sapienza' University of Rome, Italy

The presence of several sheets of the Fermi surface, in pnictides superconductors, makes the multiband character of superconductivity an unavoidable ingredient of any theoretical approach. Moreover, since the calculated electron-phonon coupling cannot account for the high values of T_c , it has been suggested that the pairing glue is provided by spin fluctuations exchanged between electrons in different bands. Thus, pnictides are expected to be somehow different from other multiband superconductors (e.g., MgB_2) where the main coupling mechanism is intraband. This scenario raises interesting questions regarding the appropriate description of SC fluctuations in a multiband system dominated by interband pairing. The issue is relevant, because fluctuating Cooper pairs above T_c contribute to several observable quantities, such as, e.g., the enhancement of dc conductivity (paraconductivity) and of the diamagnetic response as T_c is approached.

We derive the effective action for superconducting fluctuations in a two band model discussing both cases of intraband and interband dominant pairing and pointing out the emergence of a single critical mode out of a dominant interband mechanism. Then we generalize the recipe for an arbitrary number of bands. Finally we apply our procedure to a four-band model, as appropriate for pnictides and calculate the paraconductivity in two-dimensional and layered three-dimensional systems in order to compare our results with recent resistivity measurements in $SmFeAsO_{0.8}F_{0.2}$

L. Fanfarillo, L. Benfatto, S. Caprara, C. Castellani and M. Grilli, Phys.Rev.B.**79** 172508 (2009).

Mean-Field Analysis of Intra-Unit-Cell Order in the Emery Model

Mark Fisher, Eun-Ah Kim – Cornell University, USA

Motivated by recent experiments on high- T_c cuprate superconductors pointing towards intra-unit-cell order in the pseudogap phase, we investigate three distinct intra-unit-cell-ordering possibilities, namely nematic, nematic-spin-nematic, and current-loop order. We analyze the three-band Emery model of a single CuO_2 layer including various on-site and nearest-neighbor interactions within a self-consistent mean-field approach to describe and compare the microscopic origin of these different phases. We find that while the static orders in such a model both depend on a van Hove singularity and thus there is in general no coexistence, the loop current order has a different origin and can in principal coexist with nematic order.

New Correlated Model of Colossal Magnetoresistive Manganese Oxides

Denis Golosov, *Department of Physics, Bar-Ilan University, Israel*

A new minimal model is constructed for the doped manganese oxides which exhibit colossal magnetoresistance (CMR), involving broad spin-majority conduction band as well as nearly localised spin-minority electron states. A simple mean field analysis yields a temperature-dependent hybridised band structure with suppressed carrier weight at the Fermi level. Spin stiffness is complex, indicating unusually strong spin wave damping. Experimental and theoretical investigations are needed to further verify the relevance of the proposed model. Phys Rev Lett vol. **104**, 207207 (2010)

Electronic, magnetic and structural properties of $\text{Cr}_{1-x}\text{V}_x\text{N}$

Camilo Gonzalez Quintela - *University of Santiago de Compostela, Spain*

The electronic, magnetic and structural properties of stoichiometric and hole-doped CrN as well as the magnetic and electronic phase diagram for the $\text{Cr}_{1-x}\text{V}_x\text{N}$ series are reported. Stoichiometric CrN is a narrow gap, correlation-induced, semiconductor that orders antiferromagnetically below 286 K. The changes in the chemical bond associated to the magnetic order result in a non-activated behavior of the resistivity in the antiferromagnetic state, showing some similarities with other materials proposed to be itinerant-AF, like CaCrO_3 . Doping this state with holes drives the system towards itinerant electron behavior through a series of inhomogeneous magnetic/electronic states. Given the chemical and structural simplicity of this system, it could provide an interesting place to study the evolution from an antiferromagnet with a non-thermally activated charge transport to a paramagnetic metal in a non-oxide material.

Diagrammatic Monte Carlo for the Hubbard model

Jan Gukelberger, *Institute for Theoretical Physics, ETH Zurich, Switzerland*

Diagrammatic Monte Carlo (DiagMC) is a new technique for correlated fermionic systems based on sampling Feynman diagrammatic series. In contrast to conventional QMC methods, which are generally limited to small system sizes by the fermionic sign problem, DiagMC is formulated directly in the thermodynamic limit, while the sign problem is related to the diagram expansion order. The latter fact is crucial for rendering the sign problem manageable. Although so far DiagMC applications have been mostly focused on accurate determination of equations of state, the approach can be straightforwardly extended to calculating two-particle correlation functions to access phase diagrams. We describe the method for the Hubbardmodel as an instructive case and present results in two and three dimensions.

Electron spectroscopy on Strongly Correlated systems

Mahdi Hajlaoui(1), B. Mansart(1), L. Baldassarre(2), I. Lo Vecchio(3), A. Perucchi(2), S. Lupi(3), P. Dudin(2), A. Barinov(2), E. Papalazarou(1), M. Marsi(1)

(1) *Laboratoire de Physique des Solides, Université Paris-Sud, Orsay, France*

(2) *Sincrotrone Trieste, Area Science Park, Trieste, Italy*

(3) *Dipartimento di Fisica, Università di Roma "La Sapienza", Roma, Italy*

The microscopic evolution of the metal-insulator transition in Mott-Hubbard systems is one of the more important open questions in the study of strongly correlated materials. We present here our results obtained using scanning photoelectron microscopy with submi-cron spatial resolution on the prototype Mott compound V₂O₃. This system has recently attracted a lot of interest, after its multiorbital nature has been demonstrated both by experimental [1] and theoretical studies [2]. Our results clearly show the coexistence of microscopic metallic and insulator domains at the transition from the metallic to the insulating phases of the systems. The presence of these domains has already been shown to be the key to explain the peculiar properties of the paramagnetic metal-insulator transition in Cr-doped V₂O₃ [3]: the results presented here, for different doping levels, shine new light on the interplay between microscopic electronic structure and surface effects [4,5] in this model compound.

[1] J.-H. Park et al., PRB **61**, 11506 (2000) , S.-K. Mo et al., PRL **90**, 186403 (2003)

[2] G. Keller et al., PRB **70**, 205116 (2004) , A.I. Poteryaev et al., PRB **76**, 085127 (2007)

[3] S. Lupi et al., Nature Communications **1** (2010) 105

[4] F. Rodolakis et al., Phys. Rev. Lett. **102** (2009) 066805

[5] S. Borghi et al., Phys. Rev. Lett. **102** (2009) 066806

At the interface between P-type and N-type doped Mott insulator

*M. Hoek, F. Coneri, D.P. Leusink and H. Hilgenkam, University of Twente,
The Netherlands*

In this work we look into doped Mott-insulator bilayer systems as candidates for bilayer exciton studies. In particular we focus on cuprates which behave as Mott insulators for low carrier doping. Cuprates are known to have a rich phase diagram as a function of both n- and p-type doping, spanning from anti-ferromagnetism to high temperature superconductivity. This richness may be further enhanced by the possible interplay of electrons and holes at the interface between the p- and n-type materials. The cuprates are especially suitable to study this interaction, since the carrier concentration can be tuned by careful doping and bilayers can be grown epitaxially using e.g., pulsed laser deposition (PLD). Analogous to what has already been done in coupled semiconductor 2-DEG systems, we are currently exploring exciton formation in cuprate heterostructures. A tantalizing prospect is the Bose-Einstein condensation of excitonic states in these correlated electron systems, with as yet unforeseen characteristics. We focus on p-type $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$ and n-type (Nd or La) $_{2-x}\text{Ce}_x\text{CuO}_4$ bilayers with low carrier doping. Our goal is to verify whether excitons are forming at the p/n interface and to study the transport properties of the coupled p- and n-type layers. The bilayers are characterized structurally using AFM and XRD and electronically by performing Hall measurements where each layer is addressed independently.

Electronic mechanism for ferroelectricity and strong magneto-electric coupling in charge-ordered multiferroics

Leonid Isaev, Department of Physics & Astronomy, Louisiana State University, USA

We study magneto-electric phenomena in multiferroic materials, which exhibit ferroelectricity due to the charge ordering. Using rare-earth iron oxides as an example, we derive an effective model, which takes into account the Coulomb interaction, magnetic superexchange and spin-orbit effects, and is consistent with the recent X-ray absorption spectroscopy measurements in multiferroic LuFe_2O_4 . Then we demonstrate, how the interplay between quantum fluctuations and geometric frustration stabilizes the charge and ferrimagnetic spin orderings. The strong coupling, due to the double-exchange mechanism, between these orders, leads to a large magneto-electric response. Our results provide a complete physical description of the magneto-electric properties of charge-ordered multiferroics.

Numerical study of momentum dependent resonant inelastic x-ray scattering (RIXS) of cuprates.

Chunjing Jia, *Applied Physics, Stanford University, USA*

Momentum dependent resonant inelastic x-ray scattering (RIXS) is an effective probe of many-body excitations in strongly correlated materials. We perform a numerical study using cluster diagonalization technique on the momentum-resolved RIXS spectra for multi-orbital models on La_2CuO_4 . The model includes electronic orbitals necessary to highlight the nonlocal Zhang-Rice singlet, charge transfer, and d-d excitations, as well as states with apical oxygen $2p_z$ character. The substantial multi-orbital characters displayed in our calculations show good agreement with the experiments.

Theoretical and experimental work has also shown that under certain circumstances the complicated RIXS spectra can be viewed as an approximate probe of the dynamical structure factor $S(\mathbf{q}, \omega)$. We perform cluster diagonalization combined with the bi-conjugate gradient stabilized method to model the RIXS spectra and $S(\mathbf{q}, \omega)$ for the single-band Hubbard models. While these two cross sections share some similar features, there are significant quantitative differences, which highlight the qualitative distinction between these two probes.

Orbital disorder induced by charge fluctuations in vanadium Spinels

Yasuyuki Kato, Los Alamos National Laboratory, USA

We derive a low-energy model for vanadium spinels and study the evolution of orbital ordering when moving away from the deep Mott insulating regime. The underlying magnetic ordering of the Mott state leads to a rapid suppression of orbital ordering due to enhanced charge fluctuations along the ferromagnetic bonds. Orbital double-occupancy is rather low at the transition point indicating that the system is still far from a covalent regime when the orbitals become disordered.

Effects of multiple orbitals on spin-fluctuations in the ferro-pnictides

Lex Kemper - *Stanford Institute for Materials and Energy Science (SIMES) SLAC
National Accelerator Center*

The ferro-pnictides are a class of superconductor not seen before. Rapidly after their discovery, it was found that there are multiple bands of varying d-orbital character near the Fermi level. The presence of these bands requires extension of standard methodology to treat superconductors beyond the single band picture. In particular, spin-fluctuation theory, which is thought to be key in understanding the pnictides due to the presence of a nearby magnetic state, needs to be extended to allow for multiple new excitations. Here, we discuss the effect of multiple orbitals on spin-fluctuations in the pnictides, and their reflection in both the pairing state, and in the normal state resistivity and Hall effect.

“Multiorbital Spin Susceptibility in a Magnetically Ordered State - Orbital versus Excitonic Spin Density Wave Scenario”

Johannes Knolle, Max-Planck Institute, PKS, Dresden, Germany

I present a general theory of multiorbital spin waves in magnetically ordered metallic systems. Motivated by the itinerant magnetism of iron-based superconductors, we compare the magnetic excitations for two different scenarios: when the magnetic order either sets in on the on-site orbital level; or when it appears as an electron-hole pairing between different bands of electron and hole character. As an example we treat the two-orbital model for iron-based superconductors. For small magnetic moments the spin excitations look similar in both scenarios. Going to larger interactions and larger magnetic moments, the difference between both scenarios becomes striking. While in the excitonic scenario the spin waves form a closed structure over the entire Brillouin zone and the particle-hole continuum is gapped, the spin excitations in the orbital scenario can be treated as spin waves only in a close vicinity to the ordering momenta. The origin of this is a gapless electronic structure with Dirac cones which is a source of large damping. We analyze our results in connection with recent neutron scattering measurements and show that certain features of the orbital scenario with multiple order parameters can be observed experimentally.

Lattice and spin dynamics of FeSi by inelastic neutron spectroscopy

Sven Krannich - Karlsruhe Institute of Technology, Institut of Solid State Physics, Germany

FeSi is a narrow band gap semiconductor that crystalizes in the cubic B20 structure. Because of its unconventional electronic and magnetic properties, which are similar to those observed in Kondo insulators, it has often been claimed to be the first 3d system belonging to this class of materials. Though bulk properties of FeSi were studied extensively, experimental information on lattice dynamical properties of FeSi is almost absent. However, a detailed analysis of, e.g., the electronic/magnetic contribution to the specific heat is only possible with an accurate knowledge of the phonon density-of-states. Therefore, we measured the phonon dispersion along the main crystallographic directions and over the complete frequency range ($E \leq 60$ meV) at $T = 10$ K by means of inelastic neutron scattering. We compare the experimental results with theoretical calculations based on density functional theory within the local density and general gradient approximation. Further, we used scattering of polarized neutrons to search for the proposed spin gap, related to temperature induced paramagnetism in FeSi, over a large range of energy transfers and temperatures. Our data show no evidence for a spin gap up to energy transfers of 80 meV and down to $T = 15$ K. This implicates that at least the direct spin gap is larger than the charge gap measured in optical spectroscopy (73 meV).

Charge and spin order in the time domain for transition metal correlated systems

Yvonne Kung, *Physics Department, Stanford University, USA*

Using time-dependent Ginzburg-Landau theory, we study the melting and recovery of charge and spin order in transition metal correlated systems in response to an ultrashort pump pulse that destroys the stripe order. The underlying multi-orbital nature of materials such as the nickelates [ref 1] leads to coupling between the spin and charge degrees of freedom, which can only be disentangled using time-resolved resonant x-ray spectroscopy. Understanding the experimental measurements requires that we develop a theory to explain them. Solving the Gross-Pitaevskii equations for a time-dependent Ginzburg-Landau model, we explore the temporal dynamics of charge and spin order parameters and compare them to experimental observations of striped nickelates ($\text{La}_{2-x}\text{Sr}_x\text{NiO}_4$) at LCLS.

[1.] K. Tsutsui, W. Koshibae, S. Maekawa, *Phys. Rev. B* **59** (1999) 9729.

Electronic Structure of Iron-Chalcogenide Superconductors observed by Angle Resolved Photoemission Spectroscopy

Ping-Hui Lin, *Laboratoire de Spectroscopie Electronique École polytechnique fédérale de Lausanne EPFL*

Iron-chalcogenide is a special category in the iron-based superconductors. The crystal structure of members of this family is built up only with FeCh layers and the dopant atoms are usually isovalent. Recently, iron-chalcogenides have attracted a lot of attention. Compared to iron-pnictides, 11-type compounds have a relatively simpler crystal structure, a less toxic crystal growth process and the possibility of growing large single crystals. Such properties make iron-chalcogenide an ideal candidate to be studied by ARPES.

We investigate the normal state electronic structure of superconducting $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Se}_x$ by angle-resolved photoemission. A broad ARPES survey in momentum space reveals two inequivalent Fermi contours at nominally equivalent Gamma points in different Brillouin zones. The observed periodicity corresponds to a unit cell containing only one Fe atom, rather than the standard tetragonal unit cell containing two Fe atoms. We also observe a strong and selective suppression of spectral weight around the corner of the Brillouin zone.

Relating $2\Delta/T_c$ on hole Fermi surface to nodes in Iron based Superconductors

Saurabh Maiti – *University of Wisconsin, Madison, USA*

We analyze the interplay between the absence or presence of nodes in the superconducting gap along electron Fermi surfaces (FSs) in Fe pnictides and $2\Delta/T_c$ along hole FSs ($2\Delta_h/T_c$), measured by angle-resolved photoemission spectroscopy (ARPES). We solve the set of coupled gap equations for 4- and 5-pocket models of Fe pnictides and relate the presence of the nodes to $2\Delta_h/T_c$ being below a certain threshold. Using ARPES data for $2\Delta_h/T_c$, we classify various pnictides as nodal or nodeless. In particular, the classification suggests that the optimally doped $\text{Ba}_{1-x}\text{K}_x\text{Fe}_2\text{As}_2$ and $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$ are likely nodeless, but isovalent $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$ will have nodes. The classification is consistent with the current experimental picture.

Spin and Orbital Excitations Probed with Resonant Inelastic X-ray Scattering

Pasquale Marra, *IFW Dresden, Germany*

Resonant Inelastic X-ray Scattering (RIXS) has become nowadays one of the main experimental techniques to investigate elementary excitations in strongly correlated materials.

I will briefly illustrate how with RIXS one not only can determine energy but also dispersion of spin and orbital excitations.

In fact, RIXS seems to be one of the best experimental probes of dispersive orbital excitations.

Furthermore, I will show how, even in the case of pure spin excitations, RIXS is very sensitive to the symmetries of the orbitals forming the ground state.

Interplay of Spin-Orbit Coupling and Electronic Coulomb Interactions in strontium iridate (Sr₂IrO₄)

Cyril Martins - *Centre de Physique Théorique (CPhT) Ecole Polytechnique (France) et Chiba University (Japan)*

The spin-orbit interaction has been found to play a significant role in the properties of a growing variety of materials, such as the topological band insulators or the iridium-based 5d-transition metal oxides. Particularly, strontium iridate (Sr₂IrO₄) was recently described as a “spin-orbit driven Mott insulator”: according to this picture, the cooperative interaction between electronic Coulomb interactions and the spin-orbit coupling can explain the insulating state of the compound.

We have studied the paramagnetic insulating phase of this material within LDA+DMFT, a method which combines the density functional theory in the local density approximation (LDA) with dynamical mean-field theory (DMFT). Sr₂IrO₄ was found to be a Mott insulator for a reasonable value of the electronic correlations once both the spin-orbit coupling and the lattice distortions were taken into account. Moreover, our results highlight the respective roles played by these two features to reach the Mott insulating state and emphasize that only their acting together may open the Mott gap in such a compound.

Quantum Hall Edge States in Bilayer Graphene Ribbons

Victoria Mazo, *Physics department, Bar Ilan University, Israël*

We study the low energy edge states of bilayer graphene ribbons subject to a strong perpendicular magnetic field B , and show that they can be described within a continuum model (the Dirac equation). We are mainly interested in investigating the energy-band structure of ribbons with a zigzag termination. At the zero Landau Level there are eight degenerate bands, whose degeneracy can be broken and controlled by an external inter-layer voltage bias V . This leads to the opening of a gap in the bulk. On the edges, due to a mixture of hole- and particle-like bands (from the same valley), an avoided crossing occurs which can be understood within a perturbative expansion in the inter-layer hopping. On the other hand, edge states from different valleys are protected from mixing by a long-range disorder potential. Hence, hole- and particle-like states can cross without mixing, and the system has properties of a topological insulator. In the presence of interactions, the rich behavior of crossing single-electron edge states may lead to a variety of collective edge-modes, whose properties dominate the transport behavior of this system.

Field-Induced Spin-Exciton Condensation in dx_2y_2 -wave Superconductivity

Vincent Michal, V. P. Mineev – CEA Grenoble (INaC/SPSMS/Theory group), France

The implications of the spin exciton mechanism are exposed in the context of a Spin Density Wave (SDW) instability occurring inside the superconducting phase of a layered heavy electron compound. In this model a magnetic field serves as a tuning parameter bringing the system to the point where the transverse spin correlations are enhanced due to dx_2y_2 -wave superconductivity and induces an instability to a phase with coexisting superconductivity and SDW order. The model considers electrons in a crystal with antiferromagnetic interactions and provides restrictions on the Fermi surface characteristics and on the ordering wave-vector (that can be commensurate or incommensurate close to commensuration). The applications of the model are addressed to the low-temperature/high-magnetic-field phase of CeCoIn5

[M.Kenzelmann et al., Science 321, 1652 (2008), Phys. Rev. Lett. **104**, 127001 (2010)].

Why in Sr₂RuO₄ electrons in the widest band have largest mass?

Jernej Mravlje, Markus Aichhorn, Takashi Miyake, Kristjan Haule, Gabriel Kotliar –
Ecole Polytechnique, France

In multi-orbital Sr₂RuO₄ quantum oscillation and ARPES experiments unexpectedly reveal largest mass renormalization of electrons in the widest band. Origin of strong correlations in this broad (>3eV) band material with small interaction (~2eV) in extended 4d orbitals has not been understood as well. Here we, using LDA+DMFT technique relate the strong correlations to the influence of the Hund's rule coupling and the unexpected mass differentiation to the proximity of the van Hove singularity. Our theory agrees well also with NMR measurements of the temperature dependence of $1/T_1T$ and the Knight shift.

Novel electronic states in misfit cobaltates investigated by ARPES

Alessandro Nicolaou - Synchrotron SOLEIL, France

Cobaltates are a family of transition-metal oxides where metallic CoO_2 planes are intercalated with different structures, acting as charge reservoirs. Among all, sodium-cobaltates are extensively studied since the discovery of an exotic superconducting phase in $\text{Na}_x\text{CoO}_2\cdot\text{H}_2\text{O}$ in 2003. The investigation of their phase diagram as a function of doping, from the Mott-insulator limit ($x=0$) to the band insulator one ($x=1$), revealed signatures of strong correlations appearing very far from the Mott-insulator limit, for $x>0.7$. In this doping limit, good metallicity coexists with Curie-Weiss susceptibility and high thermoelectric power [*M.L. Foo et al. PRL 2004; M.Lee et al. Nat. Mat. 2006*]. Moreover, NMR and anomalous scattering experiments detect a charge order on the Co sites, with an organization dictated by the Na ordering. In order to understand what is intrinsic of the physics of the CoO_2 planes and what is instead related to the role of the Na intercalated layers, we studied the family of misfit cobaltates, where the same CoO_2 planes are intercalated with a rigid rock-salt structure [*A. Nicolaou et al. PRL 2010; A. Nicolaou et al. Europhys. Lett. 2010*].

Fe Impurity in As Tetrahedron

Tze Tzen Ong, Piers Coleman, Rutgers University, USA

The iron pnictides superconductors display a close experimental relationship between the T_c values and the tetrahedral bond angle of the As-Fe-As layer, with optimal T_c clustering close to the ideal tetrahedron geometry. In this work, we study the local moment physics of an Fe atom within an As tetrahedron, and we find that there is a strong interplay between spin and orbital degrees of freedom. The d-orbitals are crystal field split, and the lower eg orbitals have an $SU(2) \times SU(2)$ symmetry with both a spin and orbital Kondo interaction. The spin Kondo coupling is strongly reduced by the Hund's coupling, hence the system flows to an over-screened orbital Kondo state. The strong-coupling fixed point, and the leading perturbations, is studied using a Majorana fermion representation of the $SU(2) \times SU(2)$ symmetry, showing clearly how scattering from a Majorana zero mode gives rise to the resulting Marginal Fermi liquid.

We also discuss the possible implications for a superconducting instability in the pnictides.

Fermi-surface study of the iron pnictide superconductors LiFeP and LiFeAs

Carsten Putzke, *HH. Wills Physics Laboratory University of Bristol, UK*

The recently discovered 111 iron pnictide superconductors LiFeAs and its counterpart LiFeP have drawn great attention due to the fact that the material stays superconducting over the whole isovalent doping-range with $T_c \approx 18$ K for LiFeAs and $T_c \approx 5$ K for LiFeP . We present measurements of the Fermi surface carried out by de Haas-van Alphen oscillations in pulsed magnetic field up to 60T. For both endmembers we find that the data is in good agreement with conventional bandstructure calculation, with moderate renormalization of the mass. In contrast to photoemission results on LiFeAs we find that both compounds have quasi-nested Fermi surfaces.

Theory for Electron Spin Resonance in Y bAlB_4

Aline Ramires Neves de Oliveira, P. Coleman – Rutgers University, USA

In this work we propose a theory for the Electron Spin Resonance (ESR) signal in heavy fermions analysing the spin response function in the Kondo Lattice Model [1]. ESR is a powerful technique in the study for heavy-fermion systems. It is able to probe the dynamics of the localized electrons when immersed in a conduction sea. Particularly, the heavy fermion superconductor Y bAlB_4 shows an intriguing behavior when analyzed through this technique [2]. First because it is expected no ESR signal for this type of compound since the Kondo ions would have a very large broadening of the response. Second because it presents a dual character: behaving as a conduction electron or as a local moment, depending on the physical quantity analyzed.

[1] E. Abrahams, P. Wolfe, *PRB* **78**, 104423 (2008)

[2] L. M. Holanda et al., *arXiv:0908.0044v1* (2009)

Angle Resolved Photoelectron Spectroscopy and Applications

Amina Taleb-Ibrahimi – *Synchrotron SOLEIL, France*

ARPES plays an important role in characterizing the electronic properties of many advanced materials. In this poster we will report on the assets of the technique and illustrate with a panel of results obtained using the high performances of the new Cassiopée beamline at Soleil, in terms of energy, angle and spin resolution. Measured ARPES line shape in misfit cobaltates or pnictides as a function of T° and polarization which contain valuable information on the nature and importance of many body interactions in these highly correlated systems will be discussed. First direct observation of a nearly ideal graphene band structure will be demonstrated. Detailed analysis of the evolution of dispersion curves and line shape at Fermi level of heavily B-doped diamond single crystal epilayers will be reported as well as ARPES and core level measurements on alkali/Si(111) which illustrates the competition between e-e correlations and e-phonon coupling at a surface. In addition, spin polarized photoemission data on Cassiopée allowing the determination of the polarization at the Fermi level in epitaxial FeV alloys, a step toward the understanding of the transport in MgO epitaxial junctions using these alloys as electrodes, will be shown. Tailoring and modelizing novel electronic states is challenging for the fundamental physics as well as of great interest for future technological applications.

Thermal Conductivity in the ferromagnetic superconductor UCoGe

Mathieu Taupin, CEA Grenoble/INaC/SPSMS, France

More than ten years ago, the first ferromagnetic superconductor, UGe₂, was discovered. Itinerant ferromagnetic superconductors are natural candidates for multigap superconductivity, as it is expected that pairing will occur “separately”, on each Fermi surface of a given spin orientation. They also present very striking behaviors, notably under high field : superconductivity is enhanced by the magnetic field (applied in peculiar directions), with the presence of a re-entrant superconducting phase at high field. Two other compounds have been found to have the same properties at ambient pressure: URhGe in 2001 and UCoGe in 2008. This allows more quantitative experiments, in particular thermal conductivity measurements, which can probe the superconducting gap symmetry. Thermal conductivity measurements have been performed on the compound UCoGe, ferromagnetic at 2.5K and superconductor at 0.6K. It has been found that the re-entrant superconducting phase is a bulk transition and that the magnetic field has a great influence on the properties of the system when applied along the easy magnetization axis. We also discuss the influence of sample purity on the superconducting phase properties.

NMR study of magnetism and superconductivity in pnictides

Yoan Texier, J. Bobroff – Laboratoire de Physique des Solides, France

Unconventional superconductivity has now been evidenced in a wide variety of materials, high T_c cuprates, cobaltates, heavy fermions, organic conductors. Despite their differences, all these compounds share a common unexpected feature: in all their phase diagrams, superconductivity is always adjacent to a long range magnetic ordered phase, usually antiferromagnetic (AF). The Recent discovery of pnictides gives hope to understand how these two phases interact. These Fe-based materials display a spin density wave (SDW) magnetic ordering which turns into a high temperature superconductor when doping or pressure is applied. We present a ^{75}As NMR study on various pnictides family in fixed and sweep field experiments up to 14 Tesla. We study the effect of the distance between Fe-As plans on the electron behavior and superconductivity by comparing Co-doped $\text{Sr}_2\text{ScO}_3\text{FeAs}$ (1111, high inter-plan distance) and Co-doped BaFe_2As_2 (small inter-plan distance). We also study the nature of the magnetic state versus doping in electron doped $\text{Ba}(\text{Fe}_x\text{M}_{1-x})_2\text{As}_2$ (M=Co, Ni) high quality single crystals to decide whether disorder or incommensurability can explain the observed magnetic state.

Magnetism in the Kitaev-Heisenberg model with spin vacancies.

Fabien Trouselet, Giniyat Khaliullin, Peter Horsch - Max-Planck Institut
Stuttgart, Germany

We study the ground state properties of the Kitaev-Heisenberg model in a magnetic field and explore the evolution of spin correlations in the presence of non-magnetic vacancies. By means of exact diagonalizations, the phase diagram without vacancies is determined as a function of the magnetic field and the ratio between Kitaev and Heisenberg interactions. We show that in the (antiferromagnetic) stripe ordered phase the static susceptibility and its anisotropy can be described by a spin canting mechanism, accounting as well for the transition to the polarized phase when including quantum fluctuations perturbatively. Effects of spin vacancies depend sensitively on the type of the ground state. In the liquid phase, the magnetization pattern around a single vacancy in a small field is determined, and its spatial anisotropy is related to that of non-zero further neighbor correlations induced by the field and/or Heisenberg interactions. In the stripe phase, the combination of a vacancy and a small field breaks the six-fold symmetry of the model and stabilizes a particular stripe pattern. Similar symmetry-breaking effects occur even at zero field due to effective interactions between vacancies. This selection mechanism and intrinsic randomness of vacancy positions may lead to spin-glass behavior.

Raman light scattering on the $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Sex}$ and LiFeAs

Youngje Um, M. Le Tacon, M. Rahnbeck, A. Subedi, L. Boeri, C. T. Lin, P. – Max
Planck Institut, Stuttgart, Germany

The $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Sex}$ share with their pnictogen based cousins several properties: their structure is also based on a square Fe plan, the parent Fe_{1+y}Te compound is metallic, undergoes a coupled magnetic and structural transition, and becomes superconducting upon doping. This doping is achieved through Se substitution of Te at the 2c Wicoff position, and progressively suppresses magnetic ordering and structural phase transitions. Their study has recently generated a considerable interest, and significant differences with other Fe-based superconductors were rapidly revealed. Among them, the most striking are certainly the large magnetic moment ($2.5\mu_B$) and the double stripe magnetic ordering of the parent FeTe compound, to compare with the weak Fe magnetic moment in other Fe-based parent compounds (e.g. BaFe_2As_2 or LaFeAsO), in which the magnetic stripes are also rotated by 45° with respect to FeTe. To date, structural, magnetic and electronic properties have widely been investigated on $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Sex}$ superconductors, but, in contrast with other iron-based superconductors, only little work has been performed regarding lattice dynamics in these compounds. Here, I present Raman light scattering investigations of lattice dynamics on $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Sex}$. The effect of excess iron and Se concentration has been systematically investigated, with special emphasis on the Fe (B_{1g} mode), which is common to all the iron-based superconductor families. We show that this mode behavior as function of doping is very different from the one observed in other families of Fe-based superconductors, which suggests a peculiar coupling of this phonon mode to the large Fe magnetic moment in these compounds.

Volovik effect in a highly anisotropic multiband superconductor: experiment and theory

Yan Wang¹, J.S. Kim, G. R. Stewart¹, P.J. Hirschfeld¹, S. Graser², Y. Matsuda³, T. Shibauchi³, I. Vekhter⁴

1. Department of Physics, University of Florida, Gainesville, Florida 32611, USA

2. Center for Electronic Correlations and Magnetism, Institute of Physics, University of Augsburg, D-86135 Augsburg, Germany

3. Department of Physics, Kyoto University, Sakyo-ku, Kyoto 606-8502, Japan

4. Department of Physics, Louisiana State University

We present measurements of the specific heat coefficient $\delta = C/T$ in the low temperature limit as a function of an applied magnetic field for the Fe-based superconductor $\text{BaFe}_2(\text{As}_{0.7}\text{P}_{0.3})_2$. We find both a linear regime at higher fields and a limiting square root H behavior at very low fields. The crossover from a Volovik-like \sqrt{H} to a linear field dependence can be understood from a multiband calculation in the quasi classical approximation assuming gaps with different momentum dependence on the hole- and electron-like Fermi surface sheets.

Coexistence of spin density waves (SDW) and superconductivity (SC) in electron-doped cuprates

Wenya Wang, J. Knolle, I. Eremin, and P. Hirschfeld – University of Florida, USA

Some of the electron-doped cuprates exhibit a phase in the temperature-doping phase diagram where superconductivity and spin density wave order coexist at the microscopic level, and similar coexistence has been claimed in the Fe-based superconductors. To investigate the macroscopic properties of such states, we start with a one band model that predicts the behavior of Fermi surface in cuprates. By using this model and the mean-field approximation we can simulate the evolution of Fermi surfaces with different SDW order parameter (W_0).

We calculate the SC and SDW gap sizes self-consistently and the RPA susceptibility for understanding the spin exchange mechanics. We show that the RPA susceptibility changes with different W_0 in the electron-doped cuprates. We present the comparison of RPA susceptibility in the pure SDW state and these in the coexistence state of SDW and superconductivity.

Orbital selective crossovers and symmetry restoration in an asymmetric Hubbard model of cold atoms in optical lattices

Emilio Andres Winograd, *R. Chitra and M. J. Rozenberg Laboratoire de Physique des Solides, France*

We study the asymmetric Hubbard model at half-filling as a generic model to describe the physics of two species of repulsively interacting fermionic cold atoms in optical lattices. We use Dynamical Mean Field Theory to obtain the paramagnetic phase diagram of the model as function of temperature, interaction strength and hopping asymmetry.

A Mott transition with a region of two coexistent solutions is found for all nonzero values of the hopping asymmetry. In the metallic phase, a temperature driven orbital-selective crossover takes place. At low temperatures, the state is a heavy Fermi-liquid, qualitatively analogous to the Fermi liquid state of the symmetric Hubbard model. Above a coherence temperature, one fermionic species effectively localizes, and the metallic state maps onto the non-Fermi liquid of the Falicov-Kimball model.

We compute observables relevant to cold atom systems such as the double occupation, the specific heat and entropy and characterize their behavior in the different phases.

Harnessing Competition in Ferroelectric Superlattices to Engineer Enhanced Piezoelectrics

Tahir Yusufaly, Valentino Cooper, Benedikt Ziegler, Sara Callori, John Sinsheimer, Matthew Dawber, Karin Rabe and Premala Chandra, Rutgers University Department of Physics and Astronomy, USA

First-principles calculations have predicted enhanced piezoelectricity in $\text{PbTiO}_3/\text{BaTiO}_3$ superlattices beyond that of either constituent. We present further density functional studies, Landau characterization and experimental results that confirm that this is indeed the case. The numerical and the analytical calculations also successfully model the observed nonlinear behavior of the polarization and the tetragonality as a function of PbTiO_3 composition. These observed trends are shown to result from bulk electrostatics that require uniform displacement in the superlattice due to the absence of free charge. We end with a discussion of other component superlattices where these effects might be even more pronounced.

LIST OF ATTENDEES

MULTIORB 2011 - LIST OF ATTENDEES

Status	First Name	Name	Institute or Laboratory	Town, Country	email address
Organizer	Peter	Hirschfeld	University of Florida	Gainesville FL, USA	pjh@phys.ufl.edu
Organizer	Ricardo	Lobo	ESPCI, CNRS, LPEM	Paris, France	lobo@espci.fr
Organizer	Marino	Marsi	Université Paris-Sud, LPS	Orsay, France	marsi@lps.u-psud.fr
Organizer	Ilya	Vekhter	Louisiana State University	Baton Rouge LA, Usa	vekhter@lsu.edu
Lecturer	Daniel	Agterberg	University of Wisconsin Milwaukee	Milwaukee, Usa	agterber@uwm.edu
Lecturer	Henri	Alloul	Université Paris Sud, LPS	Orsay, France	henri.alloul@u-psud.fr
Lecturer	Elena	Bascones	Instituto de Ciencia de Materiales de Madrid	Madrid, Spain	leni.bascones@icmm.csic.es
Lecturer	Dmitri	Basov	University of California San Diego	La Jolla CA, Usa	dbasov@ucsd.edu
Lecturer	Cristian	Batista	Los Alamos National Laboratory	Los Alamos NM, Usa	cdb@lanl.gov
Lecturer	Silke	Biermann	CPHT, Ecole Polytechnique	Palaiseau, France	biermann@cpht.polytechnique.fr
Lecturer	Girsh	Blumberg	Rutgers, The State University of New Jersey	Piscataway NJ, Usa	girsh@physics.rutgers.edu
Lecturer	Jean-Pascal	Brison	CEA SPSMS	Grenoble, France	jean-pascal.brison@cea.fr
Lecturer	Veronique	Brouet	Universite Paris Sud, LPS	Orsay, France	veronique.brouet@u-psud.fr
Lecturer	Jure	Demsar	University of Konstanz	Konstanz, Germany	jure.demsar@uni-konstanz.de
Lecturer	Thomas	Devereaux	Stanford University, SLAC	Stanford CA, Usa	tpd@stanford.edu
Lecturer	Jennifer	Hoffman	Harvard University	Cambridge, MA, Usa	jhoffman@physics.harvard.edu
Lecturer	Adam	Kaminski	Ames Laboratory, Iowa State University	Ames IA, USA	kaminski@ameslab.gov
Lecturer	Hae Young	Kee	University of Toronto	Toronto, Canada	hykee@physics.utoronto.ca
Lecturer	Daniel	Khomskii	Koeln University	Koeln, Germany	khomskii@ph2.uni-koeln.de
Lecturer	Jerome	Lesueur	ESPCI - CNRS - UPMC	Paris, France	jerome.lesueur@espci.fr
Lecturer	Johnpierre	Paglione	University of Maryland	College Park, MD, Usa	paglione@umd.edu
Lecturer	Natalia	Perkins	University of Wisconsin-Madison	Madison WI, Usa	perkins@physics.wisc.edu
Lecturer	Florence	Rullier-Albenque	CEA, DSM/IRAMIS/SPEC/GOC	Saclay, France	florence.albenque-rullier@cea.fr
Lecturer	Jörg	Schmalian	Karlsruhe Institute of Technology	Karlsruhe, Germany	schmalian@ameslab.gov
Lecturer	Roser	Valenti	Goethe University Frankfurt	Frankfurt, Germany	valenti@itp.uni-frankfurt.de
Lecturer	Jeroen	Van Den Brink	IFW Dresden	Dresden, Germany	j.van.den.brink@ifw-dresden.de
Lecturer	Matthias	Vojta	Technischen Universitaet Dresden	Dresden, Germany	matthias.vojta@tu-dresden.de
Lecturer	Shoucheng	Zhang	Stanford University	Stanford CA, USA	sczhang@stanford.edu
Attendee	Richard	Brierley	University of Cambridge, Cavendish Lab.	Cambridge, United Kingdom	rtb28@cam.ac.uk
Attendee	Francesco	Coneri	Twente University, Mesa + Inst. Nanotech.	Enschede, The Netherlands	f.coneri@tnw.utwente.nl
Attendee	Tanmoy	Das	Los Alamos National Laboratory	Los Alamos NM, Usa	tnmydas@gmail.com
Attendee	Luca	De'Medici	CNRS, LPS	Orsay, France	demedici@lps.u-psud.fr
Attendee	Xiaoyu	Deng	CPHT, Ecole Polytechnique	Palaiseau, France	xiaoyu.deng@gmail.com

Status	First Name	Name	Institute or Laboratory	Town, Country	email address
Attendee	Laura	Fanfarillo	'Sapienza' University of Rome	Roma, Italy	Laura.Fanfarillo@roma1.infn.it
Attendee	Mark	Fischer	Cornell University, LASSP	Ithaca NY , Usa	mark.fischer@cornell.edu
Attendee	Denis	Golosov	Bar-Ilan University	Ramat-Gan, Israel	golosov@phys.huji.ac.il
Attendee	Jan	Gukelberger	ETH Zurich	Zürich, Switzerland	gukelberger@phys.ethz.ch
Attendee	Mahdi	Hajlaoui	University Paris-Sud 11, LPS	Orsay, France	mahdi.hajlaoui@u-psud.fr
Attendee	Marcel	Hoek	Twente University, Mesa + Inst. Nanotech.	Enschede, The Netherlands	m.hoek@utwente.nl
Attendee	Leonid	Isaev	Louisiana State University	Baton Rouge LA, Usa	lisaev@umail.iu.edu
Attendee	Chunjing	Jia	Stanford University, SIMES	Stanford CA, Usa	chunjing@stanford.edu
Attendee	Yasuyuki	Kato	Los Alamos National Laboratory	Los Alamos NM, Usa	ykato@lanl.gov
Attendee	Alexander	Kemper	Stanford University	Stanford CA, Usa	kemper@stanford.edu
Attendee	Johannes	Knolle	Max Planck Institute for the Physics of Complex Systems	Dresden, Germany	jknolle@pks.mpg.de
Attendee	Sven	Krannich	Karlsruhe Institute of Technology	Eggenstein, Germany	sven.krannich@kit.edu
Attendee	Yvonne	Kung	Stanford University	Stanford CA, Usa	ykung@stanford.edu
Attendee	Ping-Hui	Lin	EPFL, LES	Lausanne, Switzerland	lin.ping-hui@epfl.ch
Attendee	Saurabh	Maiti	University of Wisconsin-Madison	Madison WI, Usa	maiti@wisc.edu
Attendee	Pasquale	Marra	Leibnitz Institute, IFW	Dresden, Germany	pasquale.marra@yahoo.it
Attendee	Cyril	Martins	CPHT, Ecole Polytechnique	Palaiseau, France	cyril.martins@cpht.polytechnique.fr
Attendee	Victoria	Mazo	Bar Ilan University	Ramat Gan, Israel	victoriamazo@gmail.com
Attendee	Vincent	Michal	CEA, INAC	Grenoble, France	vincent.michal@cea.fr
Attendee	Jernej	Mravlje	CPHT, Ecole Polytechnique	Palaiseau, France	jernej.mravlje@cpht.polytechnique.fr
Attendee	Alessandro	Nicolaou	Synchrotron SOLEIL	Saint Aubin, France	alessandro.nicolaou@gmail.com
Attendee	Tzen	Ong	Rutgers University	Piscataway NJ , Usa	tzen.ong@gmail.com
Attendee	Carsten	Putzke	University of Bristol	Bristol, United Kingdom	phcmp@bris.ac.uk
Attendee	Camilo	Quintela	University of Santiago de Compostela, CIQUS	Santiago de Compostela, Spain	camiloxabier.quintela@gmail.com
Attendee	Aline	Ramires N. de	Rutgers University	Piscataway NJ, Usa	ramires@physics.rutgers.edu
Attendee	Jonathan	Ruhman	Weizmann institute of science	Rehovot, Israel	jonathan.ruhman@gmail.com
Attendee	Amina	Taleb-Ibrahim	CNRS, Synchrotron SOLEIL	St Aubin, France	amina.taleb@synchrotron-soleil.fr
Attendee	Mathieu	Taupin	CEA, INAC	Grenoble, France	mathieu.taupin@hotmail.fr
Attendee	Yoan	Texier	Université Paris sud 11	Orsay, France	yoan.texier1@u-psud.fr
Attendee	Fabien	Trousselet	Max-Planck Society	Stuttgart, Germany	f.trousselet@fkf.mpg.de
Attendee	Youngje	Um	Max-Planck Institute	Stuttgart, Germany	Y.Um@fkf.mpg.de
Attendee	Philip	Walmsley	University of Bristol, H.H. Wills Lab.	Bristol, United Kingdom	phil.walmsley@bristol.ac.uk
Attendee	Wenya	Wang	University of Florida	Gainesville FL, Usa	wwang@ufl.edu
Attendee	Yan	Wang	University of Florida	Gainesville FL, Usa	ywang@phys.ufl.edu

Status	First Name	Name	Institute or Laboratory	Town, Country	email address
Attendee	Zhong-Chao	Wei	Institute of Physics, Chinese Academy of Sciences	Beijing, China	weizhongchao@gmail.com
Attendee	Emilio	Winograd	CNRS, LPS	Orsay, France	emilio.winograd@u-psud.fr
Attendee	Jitong	Yu	University of Illinois at Urbana-Champaign	Urbana IL, Usa	jyu23@illinois.edu
Attendee	Tahir	Yusufaly	Rutgers University	Piscataway NJ, Usa	yusufaly@physics.rutgers.edu
Assist. Org.	Mehl	Nadine	CNRS, LPS	Orsay, France	mehl@lps.u-psud.fr