New physics due to Spin-Orbit coupling in CORrelated electron systems - Sciencesconf.org

	Tuesday, August 4, 2015
08:00	
	>8:30 (30min)
	Welcome
09:00	Des McMorrow: Introduction to X-ray and neutron scattering
10:00	
	>10:30 (30min) Coffee break
11:00	D. Carpentier: Topological band theory part 1
12:00	
	>12:30 (2h) Lunch break
13:00	
14:00	
	P. Coleman: Introduction to Heavy Fermions
15:00	
16:00	>16:00 (30min) Coffee break
	>16:30 (1h) Discussion time
17:00	
	>17:30 (1h30) Welcome cocktail
18:00	
19:00	

Introduction to X-ray and neutron scattering

Des McMorrow

London Centre for Nanotechnology, UCL

An introductory overview will be given of X-ray and neutron magnetic scattering. Both techniques are established as being indispensible in providing unique insight into the nature of magnetic correlations on all relevant length and energy scales. The weak scattering limit of both techniques (in contrast to the case of electrons, for example) also enables direct comparison with theory. While traditionally these techniques have been largely viewed as being complementary to one another, recent advances in X-ray methods means that there is much more direct competition.

Emphasis will be placed on the scattering cross-section, with outline derivations presented following the identification of the relevant interaction Hamiltonians for the particular scattering process under consideration. Recent developments in resonant X-ray scattering (elastic and inelastic) will be highlighted. The intention is to equip the student with enough insight to enable him or her to make an informed choice of the best technique for the particular problems of interest.

Topological band theory

David Carpentier

ENS Lyon

These lectures will provide an introduction to the notion of topological characterization of condensed matter phases within band theory. I will focus on both gapped phases and semi-metals, and will favor the illustration by simple examples to an exhaustive treatment.

Heavy Fermions and Topological Kondo insulators

Piers Coleman

Department of Physics and Astronomy, Rutgers University, Department of Physics, Royal Holloway, University of London, UK

Heavy Fermion materials are the perfect research workhorse for exploring the emergent properties of materials at the brink of magnetic instability[1]. In this two lecture course, I will provide a brief introduction to the physics of heavy fermion materials, discussing the basic models and the approximate mean-field treatments of these systems. The second lecture will focus on the effects of strong spin-orbit coupling and topological aspects of heavy fermions, introducing topological Kondo insulators[2].

References:

[1] Piers Coleman, Heavy Fermions: electrons at the edge of magnetism, Handbook of Magnetism and Advanced Magnetic Materials, 2007. arXiv:cond-mat/0612006

[2] Maxim Dzero, Jing Xia, Victor Galitski, Piers Coleman, Topological Kondo Insulators, Annual Reviews of Condensed Matter Physics, Vol 7 (2016). arXiv:1506.05635.



Session	Speech	Logistics	Break	Tour	

Experimental studies of 5d systems

Des McMorrow

London Centre for Nanotechnology, UCL

For the last fifty years the Mott-Hubbard model has served as the enduring paradigm for describing strongly-correlated electron systems, forming the basis for our understanding of hightemperature superconductors, low-dimensional quantum magnets, atomic gasses, etc.

The metal-insulator transition (MIT) it displays - driven as it is by purely electronic correlations - is one of its defining features. New classes of materials have been recently discovered that potentially fall outside of the Mott-Hubbard paradigm, offering challenges and opportunities to both experimentalists and theorists alike. These are materials characterized by strong spinorbit interaction and extended orbitals, such as are found in 4d and 5d transition metal oxides (TMO). In this talk I will present the results of experiments on several 5d TMO which establish novel classes of correlated systems displaying metal-insulator transitions (MIT) and unusual magnetic order and excitations.

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[2] Maxim Dzero, Jing Xia, Victor Galitski, Piers Coleman, Topological Kondo Insulators, Annual Reviews of Condensed Matter Physics, Vol 7 (2016). arXiv:1506.05635.

	Thursday, August 6, 2015
09:00	»9:00 (1h30) A. Santander-Syro: ARPES on 2D e. gases
	A. Santander-Syro. All ES on 2D e- gases
10:00	
	Coffee break
11:00	»11:00 (1h30) B Süsstrunk: Mechanical analogues of topological insulators
	R. Susstrunk. Mechanical analogues of topological insulators
12:00	
	Lunch break
13:00	
14.00	
14:00	
	>14:30 (1h30) Break
	BICUR
15:00	
16:00	Coffee break
	>16:30 (30min)
	Discussion time
17:00	>17:00 (1h) Poster flash
18:00	>18:00 (3h) Cocktail poster session
19:00	
20:00	
20.00	

High-resolution ARPES for the study of correlated-electron materials

Andrés F. Santander-Syro

CSNSM – Université Paris-Sud

Angle-resolved photoemission spectroscopy (ARPES) is a powerful technique to study the microscopic properties of solids. ARPES gives direct access to the band structure of a material, and provides valuable information about the many-body interactions affecting such band structure.

On the other hand, many interesting, and even open, problems in modern condensedmatter physics involve low electronic energy scales, of the order of a few meV, and temperatures of a few Kelvin. The experimental study of the electronic structure of these systems is best realized using (ultra-) high resolution ARPES at very low temperatures.

These lectures will introduce the basic aspects of high-resolution ARPES, from a synopsis of currently used instrumentation to its application in the study of various fascinating problems of correlated-electron systems. Time permitting, topics to be discussed include:

- Basic aspects of ARPES: measurement and instrumentation
- Brief overview of many-body effects and how to study them using ARPES.
- Electron-phonon coupling (and similar electron-boson couplings).
- Quasi-1D systems.
- Low- and high-TC superconductors.
- Kondo resonance and periodic Anderson lattice.
- Effects of spin-orbit coupling on the electronic structure.

Mechanical analogues of topological insulators

Roman Süsstrunk

Institute for Theoretical Physics, ETH Zürich

Electrons in solids can be characterized by topological quantum numbers. In its simplest form, this can be understood directly in the picture of the corresponding gives rise to the notion bandstructures, which of topological insulators. Stripped down to the properties of bandstructures, the non-trivial topology does not rely on fermionic properties or even on quantum mechanics. This fact was already used to engineer photonic arrays, topologically non-trivial features, such as exhibiting protected edge states. Recently this idea was further extended to systems governed by Newtons equations of motion. I will discuss how the ideas formulated in quantum mechanics can be carried over to classical mechanical meta-materials and point out why this is an exciting new direction.

	Friday, August 7, 2015
09:00	A. Santander-Syro: 2D electron gas at the surface of SrTiO3
10:00	
	>10:30 (30min) Coffee break
11:00	C. Weber: Introduction to numerical methods for correlated spin-orbit problems
12:00	
	>12:30 (2h)
13:00	
14:00	
	314:30 (1h30) B.J. Kim: Emergent magnetism and superconductivity in strongly spin-orbit coupled oxides
15:00	
16:00	>16:00 (30min) Coffee break
	>16:30 (1h) Discussion time
17:00	

		Session	Speech	Logistics	Break	Tour	
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Electronic structure of exotic states in some correlated-fermion materials: From hidden-order in URu2Si2 to spin-orbit coupled 2D electron gases in transparent oxides

Andrés F. Santander-Syro

CSNSM – Université Paris-Sud

The physics of strongly interacting fermions is the common thread in several challenging open problems at all scales. For instance, such physics is involved in the description of compact nuclear and sub-nuclear matter, in the study of the primitive Universe and the symmetry breakings leading to today's observable cosmos, in ultra-cold atomic gases in optical lattices, or in electrons in a large class of solids in which low-dimensional or correlated behavior is present.

Specifically, in transition-metal oxides (TMOs) and f-electron systems, strong correlations lead to a wide realm of phase transitions and exotic, often poorly understood, states of matter showing remarkable macroscopic properties –such as high-temperature superconductivity, large magneto-resistance, multiferroicity, or photo-catalytic behavior. To understand such novel states of matter, harness the diverse functionalities of correlated-electron materials, and guide potential applications, it is essential to comprehend their microscopic electronic structure, which is ultimately responsible for their macroscopic behavior.

In this lecture, I will present an overview of current research on the electronic structure of two paradigmatic correlated-electron systems:

(i) The heavy-fermion URu2Si2. This material presents a puzzling 'hidden-order' phase transition at THO = 17.5 K, characterized by a large entropy loss and an energy gap of about 10 meV in the density of states at the Fermi level. However, since its discovery in the 1980's, the identification of the associated broken symmetry and order parameter are still a riddle. Following our observation of a heavy-electron Fermi-surface instability occurring at the transition [1], we recently studied the changes in electronic structure symmetries, and opening of a momentum-dependent energy gap, across the transition [2, 3]. I will show how these data provide a unified microscopic picture of the large entropy loss, gap opening and Fermi-surface reconstruction inferred from thermodynamic and magneto-transport measurements.

(ii) The two-dimensional electron gases (2DEGs) at the surface of transition-metal oxides. We recently discovered how to create 2DEGs at the surface of some insulating transparent oxides [4 - 6]. I will show that one can also tailor their electronic structure and symmetries by choosing the confining surface [7, 8]. Then, I will discuss our recent observation of a giant spin splitting, of 100 meV, of bands with opposite spin chiralities in the 2DEG at the surface of SrTiO3 [9]. These results show that confined electronic states at oxide surfaces can be endowed with novel, non-trivial properties that are not simple extensions of the bulk bands, and are promising for technological applications.

- [1] Nature Physics 5, 637-641 (2009).
- [2] Phys. Rev. Lett. 110, 156404 (2013).
- [3] Nature Communications 5, 4326 (2014).
- [4] Nature 469, 189 (2011).
- [5] Phys. Rev. B 86, 121107(R) (2012).
 [6] Phys. Rev. B 92, 041106(R) (2015).
- [6] Phys. Rev. B 92, 041106(1 [7] Sci. Rep. 4, 3586 (2014).
- [7] Sci. Rep. 4, 3586 (2014). [8] Phys. Rev. Applied 1, 051002 (2014).
- [9] Nature Mater. DOI: 10.1038/NMAT4107 (2014).

Introduction to numerical methods for correlated spin-orbit problems

Cedric Weber

King's College London

We review the dynamical mean-field theory method (DMFT), a sophisticated approach to treat correlated electron problems. In the last decades, DMFT became one of the standard approach to describe subtle quantum mechanical effects in transition metal oxides (TMO). More recently, it was extended to the 5d TMO compounds, where the spin-orbit coupling plays a significant role. Here, we give an introduction to the DMFT method and its implementation for simple examples, and review some of the recent applications of DMFT to the iridates and osmates materials.

Emergent magnetism and superconductivity in strongly spin-orbit coupled oxides

B. J. Kim

Max Planck Institute for Solid State Research

Strong relativistic spin-orbit coupling present in 4d and 5d transition-metal oxides allows description of their magnetic properties in terms of pseudospins, which represent the entangled spin and orbital degrees of freedom. In this talk, I will discuss selected examples of how pseudospins can lead to novel emergent phenomena, studied using resonant x-ray scattering, inelastic neutron scattering, and angle-resolve photoemission.

i) Sr2IrO4 with pseudospins-1/2 on a square lattice realizes a low-energy effective Hamiltonian very similar to that of the high temperature superconducting cuprates. Indeed, the unique Fermiology of cuprates in the pseudogap phase—known as Fermi arcs—has been largely reproduced in electron doped Sr2IrO4. I will discuss on our recent experimental progress in the search of d-wave superconducting phase in electron-doped Sr2IrO4.

ii) Pseudospins-1/2 on a certain lattice and bonding geometry are predicted to have strong, bond-directional interactions, which lead to a potential realization of the long-sought Kitaev model with a quantum spin liquid ground state. I will discuss experimental evidence for the dominant bonddirectional interactions in a honeycomb lattice iridate Na2IrO3.

iii) Spin wave dispersion in an archetypal 4d Mott insulator Ca2RuO4 grossly deviates from that known for Heisenberg antiferromagnets, indicating a sizable unquenched orbital moment and a prominent effect of spin-orbit coupling in determining the form of magnetic interactions. I will discuss an effective model for Ca2RuO4 in terms of pseudospins derived from the microscopic Hamiltonian.



Session	Speech	Logistics	Break	Tour	

Spin-orbit Mott insulators, novel magnetic orders and spin liquids

Yong-Baek Kim

Department of Physics, University of Toronto

We discuss recent progress in understanding correlated materials with strong spin-orbit coupling. In particular, we focus on theoretical framework to understand topological phases of matter that include quantum spin liquid, topological insulators, and topological semi-metals. Novel magnetic order in spin-orbit Mott insulators proximate to the topological phases are also discussed. We consider applications of these ideas to recent experiments on various 5d transition metal oxides, especially 2D and 3D honeycomb iridates A2IrO3 as well as pyrochlore iridates R2Ir2O7.

Introduction to oxide interfaces

Andrea Caviglia

Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands

Motivation: correlated materials as opposed to conventional semiconductors.

Electronic structure of transition metal oxides.

Control methods. Epitaxial strain, charge transfer.

Synthesis methods. MBE and PLD.

Characterisation methods. X-ray scattering, TEM with EELS.

Interfaces between a Mott insulator and a band insulator: the case of LaTiO3/SrTiO3.

Interfaces between polar and non-polar insulators: the case of LaAlO3/SrTiO3.

Doping mechanism, polar discontinuity, role of defects.

Magnetism and two-dimensional superconductivity.

Superconductor-insulator transition.

Interfaces between strongly correlated oxides: nickelates heterostructures.

Electronic Structure of Iridates: a combined Density Functional Theory Dynamical Mean Field Theory Point of View

Silke Birmann

CPHT, Ecole Polytechnique

In recent years, the field of electronic structure calculations for correlated electron materials has seen great progress due to the advent of combinations of many-body theory such as dynamical mean field theory (DMFT) and density functional theory (DFT). Specifically, for iridates, combined DFT+DMFT has allowed to give a quantitative meaning to the effective single-orbital problem [1] arising in some compounds, and to obtain estimates for spectral or optical properties. In this talk, we will give an introduction to DMFT and its use in electronic structure calculations. We will focus on strategies for modelling complex oxides and discuss the notion of an effective orbital degeneracy. Current topics, such as the calculation of the effective local Coulomb interactions ("Hubbard U") will be explained [2].

[1] C. Martins, M. Aichhorn, L. Vaugier, S. Biermann, Phys. Rev. Lett. 107, 266404 (2011)
[2] L. Vaugier, H. Jiang, S. Biermann, Phys. Rev. B 86, 165105 (2012)



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Topological Crystalline Metal in Perovskite Iridates

Hae-Young Kee

Department of Physics, University of Toronto

Novel interplay of spin-orbit coupling and electron correlations in quantum materials recently has emerged as a new paradigm for correlated electron physics. In particular, Iridium oxides (Iridates) with strong spin-orbit coupling have provided an excellent playground to explore exotic phases such as Kitaev spin liquid, unconventional magnetic orderings, and topological phases. In this lecture, I will first review recent studies of layered perovskite Iridates including symmetry protected nodal line Fermi surface line in SrIrO3. Then I will present how a new topological metal dubbed topological crystalline metal appears in perovskite iridates [1], and discuss its experimental implications.

[1] Yige Chen, Yuan-Ming Lu, and Hae-Young Kee, Nature Communications 6, 6593 (2015).

	Wednesday, August 12, 2015
09:00	 S. Biermann: Electronic Structure of Iridates, a DFT+DMFT point of view
10:00	
	>10:30 (30min) Coffee break
11:00	K. Haule: Metal-Insulator Transition in Iridates in proximity to topological states, and what destabilizes Jeff=1/2 state
12:00	
10.00	>12:30 (2h) Lunch break
13:00	
14:00	
	A. Caviglia: Spin-orbit-coupling at oxide interfaces
15:00	
16:00	>16:00 (30min) Coffee break
17:00	>16:30 (1h30) H. von Lohneysen: Role of geometric frustration on magnetism and quantum criticality in correlated electron systems
18:00	>18:00 (1h) Discussion time
19:00	>19:00 (4h30) Banquet BBQ
20:00	

Electronic Structure of Iridates: a combined Density Functional Theory Dynamical Mean Field Theory Point of View

Silke Birmann

CPHT, Ecole Polytechnique

In recent years, the field of electronic structure calculations for correlated electron materials has seen great progress due to the advent of combinations of many-body theory such as dynamical mean field theory (DMFT) and density functional theory (DFT). Specifically, for iridates, combined DFT+DMFT has allowed to give a quantitative meaning to the effective single-orbital problem [1] arising in some compounds, and to obtain estimates for spectral or optical properties. In this talk, we will give an introduction to DMFT and its use in electronic structure calculations. We will focus on strategies for modelling complex oxides and discuss the notion of an effective orbital degeneracy. Current topics, such as the calculation of the effective local Coulomb interactions ("Hubbard U") will be explained [2].

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[2] L. Vaugier, H. Jiang, S. Biermann, Phys. Rev. B 86, 165105 (2012)

Metal-Insulator Transition in Iridates in proximity to topological states, and what destabilizes Jeff=1/2 state

Krjstian Haule

Rutgers, The State University of NJ

The competition between spin-orbit coupling, crystal field splitting and electron correlations with comparable magnitude gives rise to many interesting phenomena. For instance, the so-called effective J=1/2 state has been observed in many iridates compounds, Ruddlesden-Popper (RP) $Sr_{n+1}Ir_nO3_{n+1}$ and pyrochlore $RE_2Ir_2O_7$ (RE=Bi, Pr, Nd, Sm, Eu, Y) iridates, where metal-insulator transitions occur driven by the interplay of electron correlations with magnetic ordering. Using first-principles methods, for correlated solids based on density functional theory and dynamical mean field theory (DFT+DMFT), we have investigated the metal-insulator transitions in both classes of iridates. We explore the robustness of the effective J=1/2 state against band effects due to itineracy, structural distortion, and strain. We show how single-particle spectra, optical conductivities, and orbital and spin moments change with strain, and we demonstrate that the ground state can be well characterized in terms of an effective energy-dependent J=1/2 state. For RP compounds, we demonstrate that the crystal field splittings induced by local structural and hybridization are critical to understand distortions previous experimental results. For pyrochlore compounds, the total energies obtained using charge self-consistent DFT+DMFT method reveal that the all-in-all-out magnetic ordering is stable at low temperature in late rare earth pyrochlores, while a bad metallic state is found in early rare earth pyrochlores, in agreement with experiments.

Spin-orbit coupling at oxide interfaces

Andrea Caviglia

Kavli Institute of Nanoscience, Delft University of Technology, The Netherlands

Electronic structure of LaAlO3/SrTiO3. Role of spin-orbit coupling and structural distortions.

Overview of theoretical results.

Magnetotransport in the diffusive limit.

Magnetotransport in the semiclassical Boltzmann picture.

Magnetotransport in the Kondo interpretation.

Photoemission spectroscopy.

Interplay of spin-orbit coupling and superconductivity. Enhancement of critical magnetic field.

5d systems: KTaO3 and outlook on iridates.

Role of geometric frustration on magnetism and quantum criticality in correlated electron systems

Hilbert v. Löhneysen

Karlsruhe Institute of Technology, Institute for Solid State Physics, 76021 Karlsruhe

In this talk I will review some recent examples where geometric frustration, spin-orbit coupling plays a decisive role in magnetism. First, I will compare the fate of the long-wavelength helical order in the weak itinerant magnet MnSi under hydrostatic pressure at low temperatures [leading to partial magnetic order [1] compared to the temperature driven transition [2]. Mn5Si3 is a hexagonal antiferromagnet with collinear and non-collinear phases at low temperature. We observe a large topological Hall effect in the non-collinear phase [3]. Finally, the heavy-fermion compound CePdAl with distorted exhibits kagomé structure а antiferromagnetic order with 1/3 of the Ce moments not partaking in the ordering due to geometric frustration [4]. A guantum phase transition can be reached upon partial replacement of Pd by Ni [5]. I will discuss the unusual features of this transition and the possibility of a spin liquid in CePdAI.

- [1] C. Pfleiderer et a., Nature 427, 227 (2004)
- [2]. A. Hamann et al., Phys. Rev. Lett. 107, 037207 (2011)
- [3] C. Sürgers et al., Nature Comm. 5, 3400 (2014)
- [4] P. Dönni et al., J. Phys. Cond. Mat. 8, 11213 (1996)
- [5] C. Fritsch et al., Phys. Rev. B 89, 054416 (2014)

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	Thursday, August 13, 2015
09:00	^{39:00 (1h30)} Z. Hasan: Topological phases and spin-orbit effects at interfaces/in heterostructures
10:00	
	>10:30 (30min) Coffee break
11:00	K. Haule: Hexadecapole order as Chirality density wave in the "hidden order" phase of URu2Si2
12:00	
	>12:30 (2h)
13:00	
14:00	
	T. Takayama: novel iridates and 3D Dirac materials 1
15:00	
16:00	>16:00 (30min) Coffee break
	>16:30 (1h) Discussion time
17:00	

Session Speech	Logistics	Break	Tour	
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Hexadecapole order as Chirality density wave in the "hidden order" phase of URu2Si2

Krjstian Haule

Rutgers, The State University of NJ

Modern spectroscopic techniques successfully determined the type of long range order in most of solids, with one prominent exceptions, termed "the hidden order". The heavy fermion material URu2Si2 is one of a few materials ordered by the "hidden mechanism". The ab-initio Dynamical Mean Field Theory calculations for this material predicted a strange hexadecapolar order back in 2009 as a result of unusual multichannel Kondo effect, which is arrested at low temperature by the crystal field splitting. The long range order can be characterized by a complex order parameter Psi, whereby a real Psi describes the hidden order phase, and an imaginary Psi corresponds to the large moment antiferromagnetic phase, providing a unified picture of the broken symmetry phases in this material. Recently Raman spectroscopy found a clear evidence for such hexadecapolar order as it necessary involves chirality density modulation picked up by Raman signal in unsual A2g symmetry channel.

Materials overview of iridates: From quantum spin liquid to Dirac semimetal

Tomohiro Takayama

Max Planck Institute for Solid State Research

5d transition-metal oxides like iridates have recently emerged as a platform of novel electronic phases produced by the interplay between strong spin-orbit coupling, modest Coulomb interaction, electron kinetic energy and crystal field. One of the unique features of iridates is that they show totally different faces depending on their lattice network. For example, isotropic Heisenberg magnetic coupling is proposed and experimentally identified in Sr2IrO4 with corner-shared IrO6 octahedra, while highly anisotropic magnetic coupling appearing in edge-shared IrO6 network is discussed to give rise to Kitaev spin liquid.

In these lectures, I will overview the vast materials of iridates based on their crystal structures. The aim is how to see and understand their crystal structures from the simple prototypes. The materials include newly discovered ones by various synthetic techniques such as thin-film fabrication, high-pressure synthesis, and soft-chemical approach.

The first talk focuses on the perovskite and related materials, and in the second talk I will visit iridates with edge-shared IrO6 network such as 2D and 3D honeycomb, spinel and hyperkagome.



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Materials overview of iridates: From quantum spin liquid to Dirac semimetal

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