PARIS EDGE 2019

CUTTING-EDGE TOPICS IN QUANTUM MATERIALS

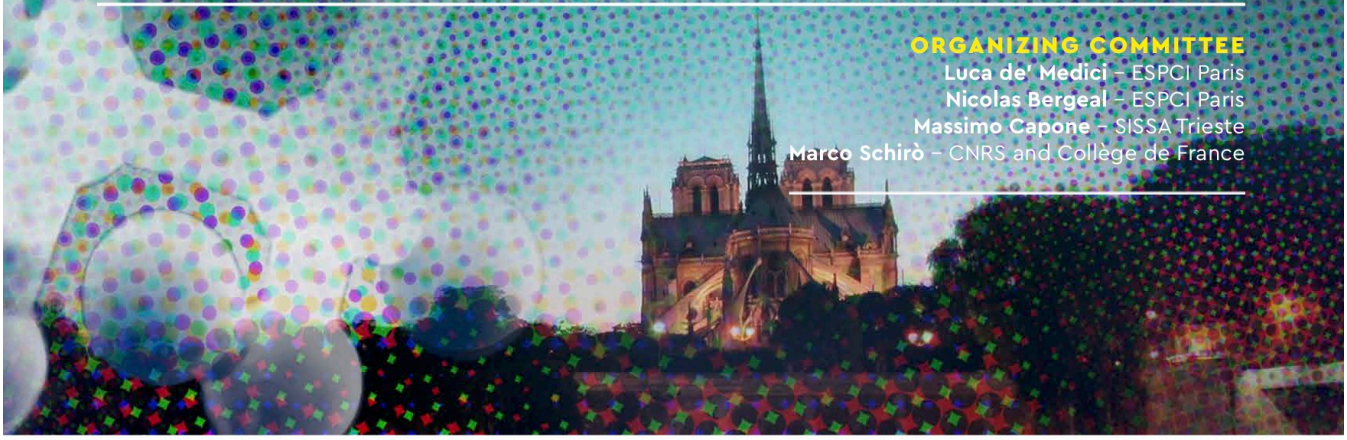
SEPTEMBER 25-28, 2019

INTERNATIONAL CONFERENCE

- HIGH-TC SUPERCONDUCTORS
- UNCONVENTIONAL METALS: THE HUND'S, THE BAD, THE HEAVY
- ENGINEERED QUANTUM MATTER: TWISTRONICS, TOPOLOGY, NON-EQUILIBRIUM
- NEW COMPUTATIONAL METHODS FOR CORRELATED SYSTEMS

INVITED SPEAKERS

Felix Baumberger – University of Geneva
Johan Biscaras – Université Pierre et Marie Curie, Paris
Lilia Boeri – Sapienza University, Rome
Matteo Calandra – Université Pierre et Marie Curie, Paris
Andrea Cavalleri – MPI Hamburg
Amalia Coldea – Oxford University
Xi Dai – Hong Kong University
Tilman Esslinger – ETH, Zurich
Benoit Fauqué – ESPCI and Collège de France, Paris
Marco Grilli – Sapienza University, Rome
Russell J. Hemley – University of Illinois, Chicago
Peter Hirschfeld – University of Florida
Nigel Hussey – High Field Magnet Laboratory, Nijmegen
Ricardo Lobo – ESPCI, Paris
Paul Loubeyre – CEA, Arpajon
Nicola Marzari – EPFL, Lausanne
Christophe Mora – ENS, Paris
Cyril Proust – LNCMI, Grenoble
Giorgio Sangiovanni – Wuerzburg University
Peter Schauss – University of Virginia
Ulrich Schollwoeck – University of Munich
Michael Sentef – MPI, Hamburg
Chandra Varma – New York University
Ali Yazdani – Princeton University



ORGANIZING COMMITTEE

Luca de' Medici – ESPCI Paris
Nicolas Bergeal – ESPCI Paris
Massimo Capone – SISSA Trieste
Marco Schirò – CNRS and Collège de France

ESPCI PARIS EDUCATION SCIENCE INNOVATION

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PARIS EDGE 2019

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- **Massimo Capone (SISSA, Trieste)**
- **Marco Schirò (CNRS and Collège de France)**

Chairing: M. Casula (U. Pierre et Marie Curie), Y. Gallais (U. Diderot), G. Sangiovanni (U. Wuerzburg), J. Lesueur (ESPCI Paris), H. Alloul (U. Paris-Sud), C. Pepin (CEA Saclay), D. Roditchev (ESPCI Paris), M. Gabay (U. Paris-Sud), M. Calandra (U. Pierre et Marie Curie), L. Boeri (Sapienza U. Rome)

Administrative help : Natasa Ilic, (ESPCI Paris), Agnès Maillard and François Laurent (Société des Amis de l'ESPCI)

The conference will be held in the :

Institut Pierre-Gilles de Gennes (IPGG), 6 rue Jean Calvin, 75005 Paris:

Conference sessions will be held in the main Amphitheater, level -1

Lunches (on the 25th and 26th) and the poster session/aperitif (25th afternoon) will be hosted in the Espace Concordia (41 rue Tournefort) just outside ESPCI and IPGG, entrance from the small nearby Place Lucien-Herr (map).

Lunch on the 27th will be held at IPGG.

Friday September 27th, 20:15.

The conference dinner-cruise (by invitation or optional reservation only) on the Seine river will be held, on Friday 27th, on the Restaurant-ship Le Capitaine Fracasse.

Invitees, please be sharp, RDV no later than 20:15 as the boat leaves (around 20:40) and, if the departure is missed, there is no further opportunity to get on board.

Access – the boat leaves from :

Ile aux Cygnes, Middle of the Bridge of Bir-Hakeim, Paris 15e arrondissement (near the Eiffel tower)

https://www.lecapitainefracasse.com/en/acces-croisiere/

Métro : Station « Bir-Hakeim » line 6 (a 5min walk from there)

If you are lost, please call the emergency/contact number +33 6 0949 3916, or the restaurant number +33 1 4141 9070.

Program

	WED 25/09	THU 26/09	FRI 27/09	SAT 28/09
08:30	registration			
08:50	opening			
09:00	Baumberger	Disa	Coldea	Hemley
09:35	Sangiovanni	Sentef	Hussey	Boeri
10:10	Chatzieleftheriou	Petocchi	Varma	Loubeyre
10:30	Isidori	Topp		
10:50	coffee break			
11:25	Lobo	Esslinger	Proust	Calandra
12:00	Casula / Lenz	Schauss	Grilli	Fauqué
12:40	Ivanshin	van Loon	Leridon	Fratini
13:00	lunch			
14:30	Marzari	Sengupta	Hirschfeld	
14:50		H Banerjee		
15:05/:10	Schollwöck	Yazdani	Bialo	
15:25			Grandadam	
15:45	coffee break			
16:20	Messio	Mora	Leroux	
16:40	van Houcke		Tocchio	
17:00	Abergel (Nature Physics)	Pizarro	Biscaras	
17:20				
17:40	Poster-aperitif		Xi Dai	
18:00				
20:15			Conference Dinner	

theoretical five-minute advance to be most likely falsified by experiments

Wednesday, September 25th

8 :50 : Opening and Welcome

SESSION 1 – chair: M. Casula (U. Pierre et Marie Curie)

9:00 : **Felix Baumberger** (U. Geneva) *Electronic correlations and enhanced spin-orbit coupling in Sr_2RuO_4 determined from high-resolution laser-based ARPES*

9:35 : **Giorgio Sangiovanni** (Wuerzburg U.) *Hund's metals respond*

10:10 : **Maria Chatzieleftheriou** (ESPCI Paris) *Enhanced electronic compressibility in a doped Mott insulator and the effect of a crystal field*

10:30 : **Aldo Isidori** (SISSA Trieste) *Charge disproportionation, mixed valence, and Janus effect in multiorbital systems: A tale of two insulators*

10 :50 : COFFEE BREAK

SESSION 2 – chair: Y. Gallais (U. Diderot)

11:25 : **Ricardo Lobo** (ESPCI Paris) *Infrared clues on the superconducting properties of Iron-Arsenide superconductors*

12:00 : **Michele Casula** (U. Pierre et Marie Curie, Paris) *Linear behavior of the optical conductivity and incoherent charge transport in $BaCoS_2$*

12:20 : **Benjamin Lenz** (U Pierre et Marie Curie, Paris) *Spectral functions of electron-doped Sr_2IrO_4 : theory vs experiment*

12:40 : **Vladimir A. Ivanshin** (U. Kazan) *Anomalous Magnetism of Pr in PrCoAsO as Studied by Electron Spin Resonance*

13:00 : LUNCH BREAK

SESSION 3 – chair: G. Sangiovanni (Wuerzburg U.)

14:30 : **Nicola Marzari** (EPFL Lausanne) *The great acceleration in computational materials discovery: a case study in 2D materials and topological insulators*

15 :05 : **Ulrich Schollwoeck** (U. Munich) *Matrix product states and real materials*

15 :45 : COFFEE BREAK

SESSION 4 – chair: G. Sangiovanni (Wuerzburg U.)

16:20 : **Laura Messio** (Sorbonne U. Paris) *High temperature expansions: up to the zero temperature! New methods of extrapolation and application to the kagome spin liquid.*

16:40 : **Kris van Houcke** (ENS Paris) *High-precision data for the unitary Fermi gas from diagrammatic series with zero convergence radius*

17:00 : **David Abergel** (associate editor at Nature Physics) *Inside Nature Physics*

17:40 – 19:30 : **POSTER SESSION** WITH APERITIF

Thursday, September 26th

SESSION 5 – chair: M. Schirò (CNRS and Collège de France)

9:00 : **Ankit Disa** (MPI Hamburg) *Driving non-equilibrium phase transitions by light-induced "strain"*

9:35 : **Michael Sentef** (MPI Hamburg) *Nonequilibrium Materials Engineering*

10:10 : **Francesco Petocchi** (U. Fribourg) *Hund excitations and the efficiency of Mott solar cells*

10:30 : **Gabriel E. Topp** (MPI Hamburg) *Topological Floquet Engineering of Twisted Bilayer Graphene*

10:50 : COFFEE BREAK

SESSION 6 – chair: M. Capone (SISSA – Trieste)

11:25 : **Tillman Esslinger** (ETH Zurich) *From Floquet engineering to dynamical gauge fields*

12:00 : **Peter Schauss** (U Virginia) *Probing dynamical properties of Fermi-Hubbard systems with a quantum gas microscope*

12:35 : **Erik van Loon** (U. Bremen) *Coulomb Engineering of two-dimensional Mott materials*

13:00 : LUNCH BREAK

SESSION 7 – chair: J. Lesueur (ESPCI Paris)

14:30 : **Shamshis Sengupta** (U. Paris-Sud) *Gate-tunable superconductivity at the interface of an $AlO_x/SrTiO_3$ heterostructure*

14:50 : **Hrishit Banerjee** (TU Graz) *Understanding the effect of exchange and correlation leading to curious ferromagnetic insulating state of $LaMnO_3$ on $SrTiO_3$*

15:10 : **Ali Yazdani** (Princeton U.*) Spectroscopic signatures of many-body correlations in magic angle twisted bilayer Graphene*

15:45 : COFFEE BREAK

SESSION 8 – chair: M. Capone (SISSA Trieste)

16:20 : **Christophe Mora** (ENS Paris) *Topology and perfect metal in trilayer moiré Graphene*

16:55 : **José M. Pizarro** (U. Bremen) *Internal screening and dielectric engineering in magic-angle twisted bilayer Graphene*

Friday, September 27th

SESSION 9 – chair: H. Alloul (U. Paris-Sud)

9:00 : **Amalia Coldea** (Oxford U.) *Anomalous transport and quenched nematic criticality in $FeSe_{1-x}S_x$*

9:35 : **Nigel Hussey** (High Field Magnet Laboratory, Nijmegen) *Effective Hall number across the strange metal regime of hole-doped cuprates*

10:10 : **Chandra Varma** (New York U.) *Linear in T and linear in |H| resistivity in cuprates, Heavy Fermions and Fe-based compounds*

10:45 : COFFEE BREAK

SESSION 10 – chair: C. Pepin (CEA Saclay)

11:30 **: Cyril Proust** (LNCMI Toulouse) *Universal T-linear Resistivity and Planckian Dissipation in Overdoped Cuprates*

12:05 : **Marco Grilli** (Sapienza U. Rome) *Dynamical Charge Density Waves pervading the phase diagram of High-T_c Superconducting Cuprates*

12:35 : **Brigitte Leridon** (ESPCI Paris) *Interplay between CDW and superconducting fluctuations: a new perspective*

13 :00 : LUNCH BREAK

SESSION 11 – chair: D. Roditchev (ESPCI Paris)

14:30 : **Peter Hirschfeld** (*U. Florida*) *From Mott to Not: Phenomenology of the Overdoped Cuprate Superconducting State*

15:05 : **Izabela Bialo** (TU Wien) *Synchrotron x-ray studies of the Charge Density Wave order*

15:25 : **Maxence Grandadam** (CEA Saclay) *Entangled preformed Cooper and Excitonic pairs in cuprate superconductors*

15 :40 : COFFEE BREAK

SESSION 12 – chair: M. Gabay (U. Paris-Sud)

16:20 : **Maxime Leroux** (LNCMI Toulouse) *Disorder raises the critical temperature of a cuprate superconductor*

16:40 : **Luca F. Tocchio** (Politecnico Torino) *Metallic and insulating stripes and their relation with superconductivity in the doped Hubbard model*

17:00 : **Johan Biscaras** (U. Pierre et Marie Curie Paris) *Tuning superconductivity in atomically thin materials with space charge doping*

17:35 : **Xi Dai** (Hong-Kong U.) *Pseudo Landau levels, non-local exchange and quantum anomalous Hall effect in twisted bi-layer Graphene systems*

20:15 CONFERENCE DINNER (upon invitation or optional reservation only)

Saturday, September 28th

SESSION 13 – chair: M. Calandra (U. Pierre et Marie Curie Paris)

9:00 : **Russel J. Hemley** (U. Illinois Chicago) *High-Tc Superconductivity in Dense Hydrogen Systems*

9:35 : **Lilia Boeri** (“Sapienza” U. Rome) *High-Tc Superconductivity at High Pressures*

10:10 : **Paul Loubeyre** (CEA Arpajon) *Observation of the transition to metal hydrogen: a stepping stone towards disclosing novel quantum many-body effects*

10:45 : COFFEE BREAK

SESSION 14 – chair: L. Boeri (“Sapienza” U. Rome)

11:30 : **Matteo Calandra** (U. Pierre et Marie Curie Paris) *Crystal prediction in dense hydrogen systems: the crucial role of quantum ionic effects*

12:00 : **Benoit Fauqué** (ESPCI and Collège de France Paris) *Metallicity driven by thermal amplification of the carrier mass in $SrTiO_3$*

12:35 : **Simone Fratini** (CNRS Grenoble) *Unconventional electronic transport from the scattering off slow bosons*

POSTER SESSION on Wednesday 25th, 17:40 – 19:30

Book of Abstracts: invited and contributed talks

Wednesday September 25th

Electronic correlations and enhanced spin-orbit coupling in Sr_2RuO_4 determined from high-resolution laser-based ARPES

Felix Baumberger[1,2], Anna Tamai[1], Manuel Zingl[3], Antoine Georges[3,4,5,1]

[1]*Department of Quantum Matter Physics, University of Geneva, Switzerland*
[2]*Swiss Light Source, PSI, Switzerland*
[3]*CCQP, Flatiron Institute, New York, USA*
[4]*Centre de Physique Théorique, CNRS, Ecole Polytechnique, Paris, France*
[5]*Collège de France, Paris, France*

We combine laser-based angle-resolved photoemission and dynamical mean-field theory calculations to study the interplay of electron-electron correlations and spin-orbit coupling (SOC) in the model Fermi liquid Sr_2RuO_4. Analyzing the experimental Fermi surface, we show that correlations enhance SOC by a factor of ~2 over the bare value. We further reveal that the real part of the self-energy of the β and γ sheet is momentum dependent and strongly non-linear down to low energies, in contrast to widely held believes about the phenomenology of Fermi liquids. Introducing a new method to determine orbital self-energies from quasiparticle states with multi-orbital composition, we demonstrate that the anisotropy of the self-energy does not imply momentum dependent many-body interactions. The non-linearity of the self-energy is reproduced by single-site dynamical mean field theory, which provides strong evidence for a dominantly electronic origin of 'kinks' in the quasiparticle dispersion of Sr_2RuO_4.

Hund's Metals Respond

Giorgio Sangiovanni[1]

[1]*Wuerzburg University*

The talk focuses on the spin and charge response functions of Hund's metals. I will first discuss the case of two Osmium oxides that, notwithstanding their delocalized 5d-orbitals, we claim to be unexpectedly close to a Mott transition. Then I will turn to the iron-based superconductors and analyze the real-time spin dynamics associated to the screening of the Hund's coupling-driven local moments. Within DFT+DMFT we find an enhancement of the compressibility upon approaching integer filling, pointing at the presence of a charge instability in this class of Hund's metals.

Enhanced electronic compressibility in a doped Mott insulator and the effect of a crystal field

Maria Chatzieleftheriou[1], Maja Berovic[2], Pablo Villar Arribi[1], Massimo Capone[2], Luca de' Medici[1]

[1] LPEM, ESPCI Paris, PSL Research University, CNRS, Sorbonne Université, 75005 Paris, France
[2] International School for Advanced Studies (SISSA), Via Bonomea 265, I-34136 Trieste, Italy

It is known that a doped half-filled Mott insulator, in presence of Hund's coupling, exhibits a crossover between a normal metal and a Hund's metal. It has also been shown that near this frontier an enhancement of the electronic compressibility is found, culminating in a divergence, possibly related to the mechanism for high-Tc superconductivity. We explore the effect of a crystal field removing the orbital degeneracy on the zone of enhanced compressibility and we find that it results in an extension of the instability zone towards larger dopings, placing it close to the region of parent compounds of the Fe-based superconductors.

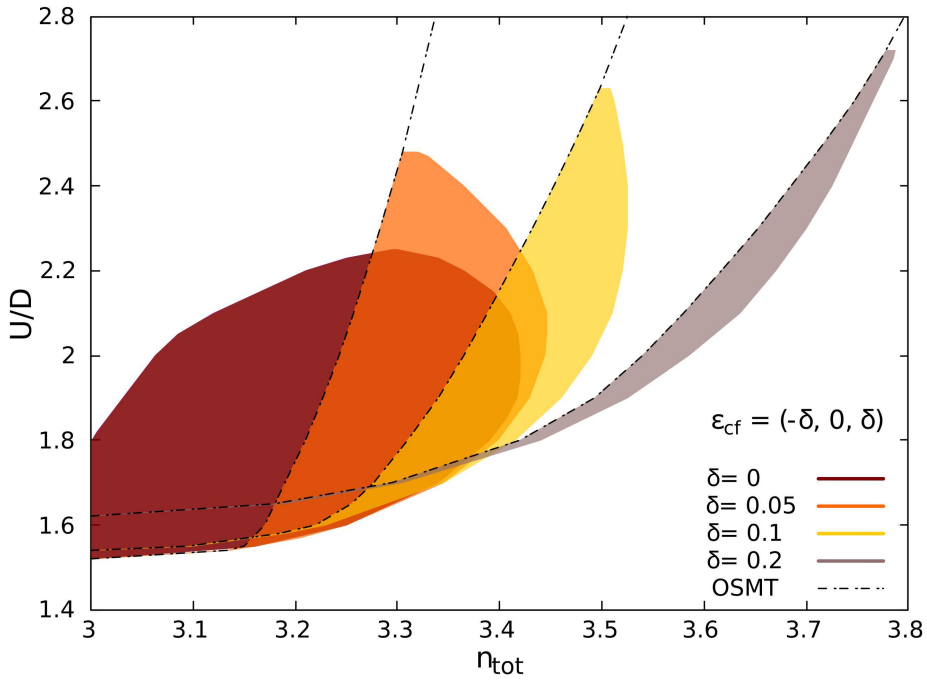

Figure 1: Zone of instability towards phase separation in a 3-band model with crystal field

Charge disproportionation, mixed valence, and Janus effect in multiorbital systems: A tale of two insulators

Aldo Isidori[1], Maja Berovic[1], Laura Fanfarillo[1], Luca de' Medici[2], Michele Fabrizio[1], Massimo Capone[1],

[1] *SISSA (Scuola Internazionale Superiore di Studi Avanzati), Trieste, Italy*
[2] *Laboratoire de Physique et d'Etude des Materiaux, ESPCI Paris, France*

Multiorbital Hubbard models host strongly correlated "Hund's metals" even for interactions much stronger than the bandwidth. We characterize this interaction-resilient metal as a mixed-valence state. In particular, it can be pictured as a bridge between two strongly correlated insulators: a high-spin Mott insulator and a charge-disproportionated insulator which is stabilized by a very large Hund's coupling. This picture is confirmed by comparing models with negative and positive Hund's coupling for different fillings. Our results [1] provide a characterization of the Hund's metal state and connect its presence with charge disproportionation, which has been recently observed in chromates and proposed to play a role in iron-based superconductors.

References

1. **A. Isidori et al., Phys. Rev. Lett. 122, 186401 (2019)**

Infrared clues on the superconducting properties of Iron-Arsenide superconductors

R.P.S.M. Lobo[1,2]

[1] *LPEM, ESPCI Paris, PSL University, CNRS,Paris, F-75005*
[2] *Sorbonne Université, CNRS, LPEM, Paris, F-75005*

The nature of the superconducting mechanism in iron-arsenide superconductors has a complex combination of electronic and lattice signatures. Superconductivity competes and cooperates with magnetic orders and responds in diverse ways to impurites and doping. Here I will cover the optical conductivity signatures of the superconducting transition in the phase diagram of $(Ba,K)Fe_2As_2$. The optimally doped material shows a fully developed superconducting gap. However, in-gap states appear when one moves towards the underdoped regime. These states appear simultaneously to the normal state spin-density-wave phase [1], indicating a strong interplay between magnetism and superconductivity. Concomitantly, the same series shows a electron-phonon coupling with a phonon Fano asymmetry that scales with the superconducting transition temperature [2]. I will discuss these results in the perspective of the gap symmetry and the superconducting pairing.

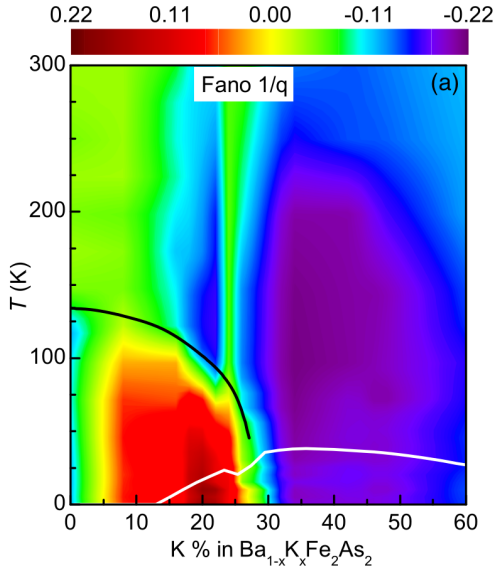

Figure 1: Fano asymmetry parameter throughout the (Ba,K)Fe_2As_2 phase diagram.

References

1. **B. Xu *et al.*, "Infrared probe of the gap evolution across the phase diagram of $Ba_{1-x}K_xFe_2As_2$" Phys. Rev. B 96, 115125 (2017).**
2. **B. Xu *et al.*, "Scaling of the Fano effect of the in-plane Fe-As phonon and the superconducting critical temperature in $Ba_{1-x}K_xFe_2As_2$", Phys. Rev. Letters 122, 217002 (2019).**

Linear behavior of the optical conductivity and incoherent charge transport in $BaCoS_2$

D. Santos-Cottin,[1,2] Y. Klein,[3] Ph. Werner,[4] T. Miyake,[5] L. de' Medici,[1,2] A. Gauzzi,[3] R. P. S. M. Lobo,[1,2] and M. Casula[3,*]

[1] *LPEM, ESPCI Paris, PSL University; CNRS; 10 rue Vauquelin, F-75005 Paris, France*
[2] *Sorbonne Université; CNRS; LPEM; F-75005 Paris, France*
[3] *Institut de Minéralogie, de Physique des Matériaux et de Cosmochimie (IMPMC), Sorbonne Université, CNRS UMR 7590, IRD UMR 206, MNHN; F-75252 Paris, France*
[4] *Department of Physics, University of Fribourg, 1700 Fribourg, Switzerland*
[5] *Research Center for Computational Design of Advanced Functional Materials, AIST, Tsukuba 305-8568, Japan*

Optical conductivity measurements on a BaCoS2 single crystal unveil an unusual linear behavior over a broad spectral range. In the paramagnetic phase above 300 K, ab initio dynamical mean field theory calculations including a retarded Hubbard interaction explain the data in terms of an incipient opening

of a Co(3d)-S(3p) charge-transfer gap concomitant to incoherent charge transport driven by electronic correlations. These results point to a non-Fermi liquid scenario with Hund's metal properties in the paramagnetic state, which arises from an incipient Mott phase destabilized by low-energy charge fluctuations across the vanishing 3d-3p charge-transfer gap [1]. This is in contrast with previously proposed scenario of a charge-transfer Mott insulator.

References

1. **D. Santos-Cottin *et al.*, Phys. Rev. Mat. 2, 105001 (2018)**

Spectral functions of electron-doped Sr_2IrO_4 : theory vs experiment

Cyril Martins [1], Benjamin Lenz [2], Silke Biermann [2,3]

[1] LCPQ, CNRS, Université Toulouse III Paul Sabatier, Toulouse, France [2] CPHT, CNRS, Institut Polytechnique de Paris, Palaiseau, France [3] Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France

The spin–orbit Mott insulator Sr_2IrO_4 has attracted a lot of interest in recent years from theory and experiment due to its close connection to isostructural high-temperature copper oxide superconductors. Despite of not being superconducting, its spectral features closely resemble those of the cuprates, including Fermi surface and pseudogap properties.
We study the evolution of the electronic structure of Sr_2IrO_4 upon doping using a combination of ab-initio density functional theory and a cluster extension of dynamical mean-field theory (" oriented-cluster DMFT "). We compare our results with recent photoemission data and find good agreement with experiment. [1]

References

1. **B Lenz *et al* 2019 *J. Phys.: Condens. Matter* 31 293001 (2019)**

Anomalous Magnetism of Pr in PrCoAsO as Studied by Electron Spin Resonance

V.A. Ivanshin[1,2], H.-A. Krug von Nidda[3], A. Loidl[3], V.P.S. Awana[4,5]

[1] Kazan Federal (Volga region) University, Kremlevskaya Str. 18, 420008 Kazan, Russia
[2] Kazan State Power Engineering University, 51 Krasnoselskaya Str., 420066 Kazan, Russia
[3] Experimental Physics V, Center for Electronic Correlations and Magnetism, University of Augsburg, 86135 Augsburg, Germany

[4] *National Physical Laboratory (CSIR), Dr. K. S. Krishnan Road, New Delhi-110012, India*

[5] *Academy of Scientific and Innovative Research (AcSIR), NPL, New Delhi-110012, India*

We have studied the itinerant ferromagnet PrCoAsO by means of electron spin resonance (ESR) spectroscopy in a broad temperature range between 4 and 300 K. ESR study demonstrates that Pr exhibits anomalous behavior in PrCoAsO, as the same though magnetic but still behaves more closely with non-magnetic La counterpart LaCoAsO than the magnetic rare earth (RE) comprising Sm/Nd/GdCoAsO. In FM phase, due to delocalization of electrons in presence of low external magnetic fields, conductivity increases quadratically as this is the case of paramagnetic phase. We suppose that RE ions influence the FM phase only via the induced structural shrinkage without involving any active role from the electronic f degrees of freedom, which are only giving a sizable magnetic contribution at much lower temperatures [1].

References

1. **G. Prando *et al.,* Phys. Rev. B 92, 144414 (2015)**

The great acceleration in computational materials discovery: a case study in 2D materials and topological insulators

Marzari N.[1]

[1] *EPFL, Lausanne*

First-principles simulations are one of the greatest current accelerators in the world of science and technology, thanks to a sustained worldwide push for ideas, algorithms and codes to model complex materials properties, underwritten by hardware that has been doubling in capacity every 14 months for the past 30 years.

I'll highlight some of my own perspectives on this, taking as a case study the discovery of novel two-dimensional materials and of their properties and applications, where we have performed an extensive high-throughput screening of known inorganic materials in order to identify those that could be exfoliated into novel two-dimensional monolayers and multilayers, followed by a thorough characterization of their properties.

Thanks to the use of the AiiDA (http://aiida.net) materials' informatics platform, all calculations are performed in fully searchable and reproducible ways, stored with the full provenance tree of all parent and children calculations, and shared with the community at large in the form of raw or curated data via the Materials Cloud (http://www.materialscloud.org) dissemination portal.

Matrix product states and real materials

Schollwöck U[1]

[1] *LMU Munich*

Tensor-network-based methods, in particular matrix product state algorithms, have been extremely successful in the simulation of low-dimensional model Hamiltonians in and out of equilibrium. Yet, the gap to real materials as treated in e.g. the DFT world has not really been bridged. Building this bridge is an ongoing effort in the context of providing impurity solvers for DMFT and DCA combined with realistic DFT band structures, applied to strongly correlated materials. I will briefly review the field and present DMFT calculations using an imaginary-time MPS solver on a real DFT band structure for off-diagonal self-energies due to the presence of spin-orbit coupling, in a situation where CTQMC faces a sign problem. There is no fitting or phenomenological modelling. I will also discuss the perspectives of this type of methods for the future.

High temperature expansions: up to the zero temperature ! New methods of extrapolation and application to the kagome spin liquid.

Laura Messio[1], Bernard Bernu[1], Laurent Pierre[2], Karim Essafi[1]

[1] *LPTMC, Sorbonne Université, Paris.*
[2] *Université de Nanterre*

If the ground state of the S=1/2 kagome antiferromagnet (KAF) is now recognized as a spin liquid (SL), its exact nature remains unprecise, even if more and more clues are in favor of a gapless SL. We use high temperature series expansions (HTSE) to propose an evolution of the specific heat and of the magnetic susceptibility with respect to temperature, for two different types of gapless SL (linear and quadratic low T specific heat). HTSE calculate exactly the first Taylor coefficients (in powers of beta=1/T) of thermodynamic functions. These quantities are then extrapolated over the full range of temperature using the entropy method[2]. We get HTSE up to order 20 in beta and calculate the coefficients as exact functions of the magnetic field. We extrapolate thermodynamical quantities for various perturbations of the ideal Heisenberg Hamiltonian: Ising anisotropy, randomly distributed site vacancies (see Figure 1), Dzyaloshinskii-Moriya, second and first neighbors interactions.

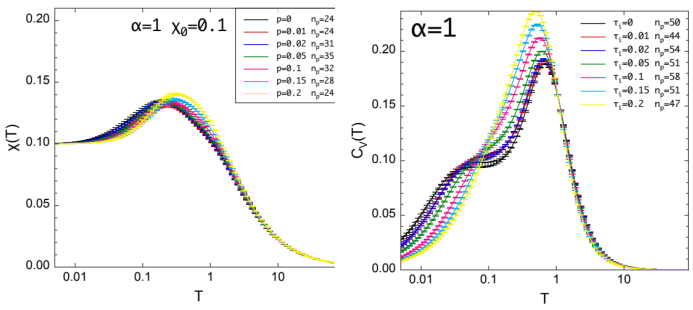

Figure 1: Effect of spin vacancies on the magnetic susceptibility and on the specific heat of

the kagome antiferromagnet (results of high temperature series expansions to order 20).

References

1. **B. Bernu, L. Pierre, K. Essafi and L. Messio, in preparation.**
2. **B. Bernu and C. Lhuillier, Phys. Rev. Lett. 114, 057201 (2015)**

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High-precision data for the unitary Fermi gas from diagrammatic series with zero convergence radius

Riccardo Rossi[1], Takahiro Ohgoe[2], Kris Van Houcke[3], Félix Werner[4]

[1] Center for Computational Quantum Physics, Flatiron Institute, 162 Fifth Avenue, New York, NY 10010, USA
[2] Department of Applied Physics, University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-8656, Japan
[3] Laboratoire de Physique de l'Ecole Normale Supérieure – Université PSL, CNRS, Sorbonne Université, Université Paris-Diderot, Paris, France
[4] Laboratoire Kastler Brossel, Ecole Normale Supérieure – Université PSL, CNRS, Sorbonne Université, Collège de France, Paris, France

We consider the unitary Fermi gas (spin 1/2 fermions with contact interactions in 3D, which describes cold atomic gases at a Feshbach resonance) in the normal phase. Thanks to a diagrammatic Monte Carlo algorithm, we accurately sample all skeleton diagrams (built on dressed single-particle and pair propagators) up to order nine [1]. The diagrammatic series is divergent and there is no small parameter so that a resummation method is needed. We compute the large-order asymptotics of the diagrammatic series, based on a functional integral representation of the skeleton series and the saddle-point method. We show that the radius of convergence is actually zero, but the series is still resummable, by a generalised conformal-Borel transformation that incorporates the large-order asymptotics [2]. This yields new high-precision data, not only for the equation of state, but also for Tan's contact coefficient and for the momentum distribution [3]. We will also highlight some recent developments in (determinant) diagrammatic Monte Carlo and present new high-precision data for the Fermi polaron, which is a single impurity atom immersed in a Fermi sea.

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Book of Abstracts: invited and contributed talks

Thursday September 26th

Driving non-equilibrium phase transitions by light-induced "strain"

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Static strain is used to engineer electronic behavior in correlated materials by structurally altering microscopic interactions. Epitaxial strain, for instance, can stabilize ferroelectric or magnetic phases and tune electrical conductivity in ultrathin oxide films. Using light to dynamically exploit strain would provide a pathway to control non-equilibrium phase transitions on ultrafast timescales. Here, I show that ultrafast strain can be coherently driven by nonlinear phonon excitation and demonstrate how this leads to light-induced symmetry breaking in different materials systems [1]. In particular, I discuss two of our recent experiments exemplifying this approach. We generate metastable ferroelectricity in the "quantum paraelectric" $SrTiO_3$ by the flexoelectric coupling to optically driven strain [2], and we realize a long-lived ferrimagnetic state in an antiferromagnetic crystal using the dynamical piezomagnetic effect. The use of light to mimic strain effects enables the rational design of non-equilibrium functional properties and could be combined with heterostructures to access new hidden phases in quantum materials.

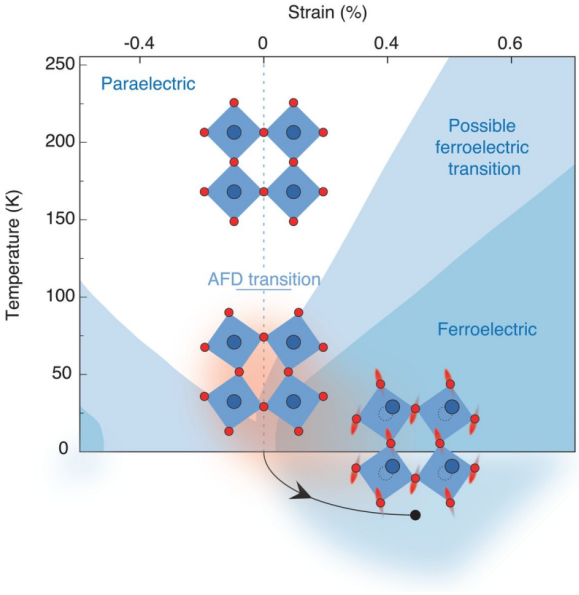

Figure 1: Schematic depiction of a dynamical ferroelectric phase transition in $SrTiO_3$ by vibrationally driven strain. From Ref. [2].

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Nonequilibrium Materials Engineering

Michael A. Sentef[1]

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The interaction of light and matter is at the heart of spectroscopies in condensed matter. With the development of ultra-short and ultra-strong laser pulses for pump-probe experiments, light is transforming from a tool to probe towards a tool to control and manipulate quantum many-body systems while driving them far away from their thermal equilibrium. In my presentation, I will discuss our recent theoretical and computational progress towards a microscopic understanding of light-driven solids with the long-term vision of nonequilibrium materials engineering.
First I will present a study on ultrafast optical control of chiral Majorana modes in topological superconductors [1], in which we present a pump pulse protocol allows for optical switching of an order parameter purely on symmetry grounds, which implies that it works both in the high-frequency („Floquet“) and low-frequency limits. Then I will show results for a cavity quantum-electrodynamical modification of electron-phonon coupling and superconductivity in monolayer FeSe/SrTiO [2], in which the pure vacuum fluctuations of a confined photon field are used to engineer materials properties.

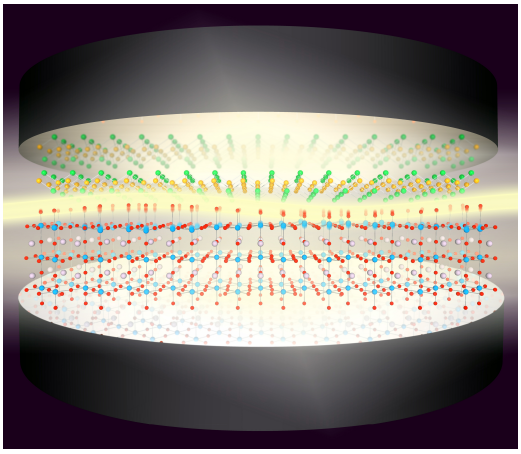

Fig.1. Illustration of 2D material monolayer FeSe on SrTiO3 substrate in a cavity [2]. (c) Jörg M. Harms, MPSD Hamburg

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Hund excitations and the efficiency of Mott solar cells

Francesco Petocchi[1], Sophie Beck[2], Claude Ederer[2] and Philipp Werner[1]

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[2] *Materials Theory, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zurich, Switzerland*

The development of photovoltaic technologies is essential for a sustainable energy production. The development of efficient solar energy conversion platforms, from semiconductors to halide perovskite, is currently the focus of many researchers, but practical issues like stability and toxicity still need to be solved. Much less in the spotlight, but conceptually interesting, is the proposal to build solar cells which exploit the strongly interacting nature of electrons in Mott insulators [1]. Charge carriers with high kinetic energy in small-gap Mott insulators can excite additional electrons across the gap via impact ionization providing a mechanism for harvesting high-energy photons, which may potentially lift the efficiency of Mott insulating solar cells above the Shockley-Queisser limit [2]. A promising system, based on $LaVO_3$, was identified by Assmann et al. in Ref. [3]. To properly assess the characteristics of Mott-based devices, we study the dynamics of photo-induced charge carriers in realistic models of $LaVO_3$ and YTO_3 polar heterostructures. We show that carrier multiplication processes, induced by local spin state transitions, occurs on the 10 fs timescale. The latter is significantly shorter compared to decay processes associated with phonon excitations, so that impact ionization should indeed contribute to the efficient harvesting of solar energy in Mott systems. As a consequence, the optimal gap size for Mott solar cells is substantially smaller than for semiconductor devices.

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Topological Floquet Engineering of Twisted Bilayer Graphene

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In twisted bilayer graphene, the electronic bandwidth and the Fermi velocity of the Dirac bands can be tuned by changing the twist angle. This leads to flat bands at particular magic angles and opens the possibility of twistronics [1] and tunable energy absorption spectra [2]. In our work [3], we investigate the topological properties of twisted bilayer graphene for an intermediate twisting angle in and out of

equilibrium on the basis of a tight-binding model. By breaking time-reversal symmetry with a circularly polarized light field, we induced a transition to a topologically non-trivial Floquet band structure with Berry curvature analogous to a Chern insulator. Thereby, the opportunity to break inversion symmetry by backgating allows to tune the phase transition between topologically trivial and nontrivial states.

From Floquet engineering to dynamical gauge fields

Esslinger T.[1]

[1] *ETH Zurich*

The coupling between gauge and matter fields plays an important role in many models of high-energy and condensed matter physics. In these models, the gauge fields are dynamical quantum degrees of freedom in the sense that they are influenced by the spatial configuration and motion of the matter field. So far, synthetic magnetic fields for atoms in optical lattices were intrinsically classical, as these did not feature back-action from the atoms. I will report on a scheme realizing the fundamental ingredient for a density-dependent gauge field by engineering non-trivial Peierls phases that depend on the site occupation of fermions in a Hubbard model. Our scheme relies on breaking time-reversal symmetry by driving the optical lattice simultaneously at two frequencies. In the experiment we quantify the amplitude of the resulting density-assisted tunnelling matrix element on a Hubbard dimer and directly measure its Peierls phase with respect to the single-particle hopping. I will further show that we can engineer the magnetic properties of a strongly interacting Fermi gas in the lattice by combining a Floquet drive with tunable interactions between the atoms [2].

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Probing dynamical properties of Fermi-Hubbard systems with a quantum gas microscope

Schauss P.[1]

[1] *University of Virginia*

The normal state of high-temperature superconductors exhibits anomalous transport and spectral properties that are poorly understood. Cold atoms in optical lattices have been used to realize the Fermi-Hubbard model, widely believed to capture the essential physics of these materials. The recent development of fermionic quantum gas microscopes has enabled the study of Hubbard systems with single-site resolution. Most studies have focused on probing equal-time spin and density correlations. In this talk, I will report on using a quantum gas microscope to probe response functions associated with unequal-time correlations relevant for understanding the pseudogap and strange metal regimes of

Fermi-Hubbard systems. First, I will describe the development of a technique to measure microscopic diffusion, and hence resistivity, in doped Mott insulators. We observed T-linear resistivity and a violation of the Mott-Ioffe-Regel limit, two signatures of strange metallic behavior. Next, I will report on the development of angle-resolved photoemission spectroscopy (ARPES) for Hubbard systems and its application to studying pseudogap physics in an attractive Hubbard system across the BEC-BCS crossover, setting the stage for future studies of the pseudogap regime in repulsive Hubbard system

Coulomb Engineering of two-dimensional Mott materials

Erik van Loon[1,2], Malte Schüler[1,2], Daniel Springer[3], Giorgio Sangiovanni[4], Jan Tomczak[3], Tim Wehling[1,2]

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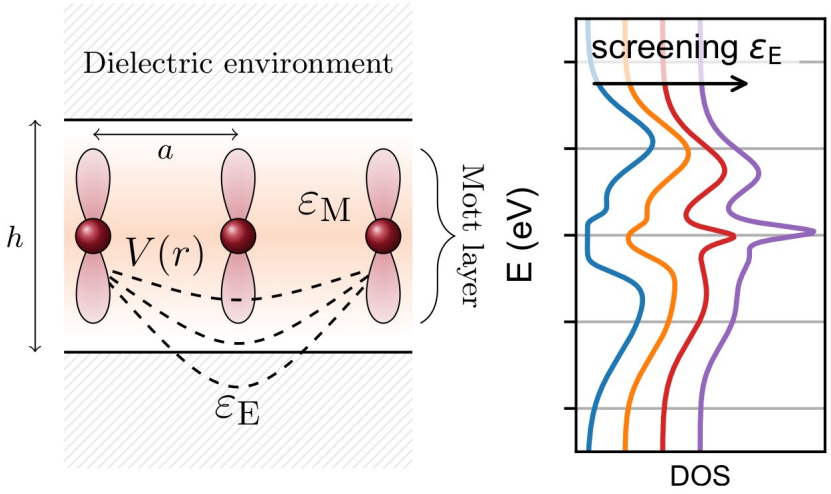
[4] *Universität Würzburg, Würzburg, Germany*

Two-dimensional materials are greatly influenced by their surroundings. Here, we show how the dielectric environment can be used to manipulate two-dimensional Mott materials. The environment directly addresses the Coulomb interaction responsible for the gap and sufficiently strong screening can turn the Mott insulator metallic. Based on our theoretical analysis, we discuss prerequisites for effective Coulomb engineering.



Gate-tunable superconductivity at the interface of an AlOx/SrTiO3 heterostructure

Shamashis Sengupta,[1] Emilie Tisserond,[2] Florence Linez,[3] Miguel Monteverde,[2] Tobias Roedel,[1] Anil Murani,[2] Philippe Lecoeur,[3] Thomas Maroutian,[3] Claire Marrache-Kikuchi,[1] Andrés F. Santander-Syro,[1] Franck Fortuna[1]

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In recent years, two-dimensional electron gases (2DEGs) in oxide-based heterostructures have emerged as model systems to probe different aspects of low-dimensional superconductivity. The carrier density of the 2DEGs can be tuned using the principle of a field-effect-transistor, allowing us to observe the evolution of electronic states as a function of electron density. We have devised a method for the facile realization of a 2DEG by the creation of oxygen vacancies [1]. The deposition in ultrahigh vacuum of a thin layer of metallic Al on SrTiO3 leads to the creation of a 2DEG due to the withdrawal of oxygen atoms from the surface by the reducing agent Al (which turns into insulating AlOx). Transport experiments reveal a 'superconducting dome' in the phase diagram. Application of a magnetic field leads to a transition between superconducting and insulating states [2]. The possibility of continuously varying the carrier density allows us to study different equilibrium and non-equilibrium features characterizing the electronic phases.

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Understanding the effect of exchange and correlation leading to curious ferromagnetic insulating state of $LaMnO_3$ on $SrTiO_3$

Hrishit Banerjee[1], Oleg Janson[2,3], Karsten Held,[3] Tanusri Saha Dasgupta[4]

[1] Institut fur Theoretische Physik – Computational Physics, TU Graz
[2] Institute for Solid State Physics, IFW, Dresden
[3] Institut fur festkorperphysik, TU Wien
[4] Indian Association for the Cultivation of Science, Kolkata.

The exotic case of the experimental observation of a ferromagnetic insulating ground state in interfaces formed by heterostructures of $LaMnO_3$ (LMO) and $SrTiO_3$ (STO) has puzzled theorists and

experimentalists[1] [2] alike. There has been some suggestions to the origin of this behaviour from the perspective of symmetry breaking and orbital ordering [3], however it does not provide a satisfactory explanation. In this study, using 3 different computational methods, DFT+Hubbard U, Hybrid DFT+Hartree Fock (HF) and DFT+DMFT calculations, we aim to show the effect of electronic exchange and correlation in driving a ferromagnetic insulating state in LMO/STO interfaces, due to electronic instabilites arising in the system, which also gives rise to charge disproportionation leading to an insulating state, which is not captured correctly by purely DFT based methods, and one requires the use of hybrid Hartree Fock exchange functionals and DMFT models to correctly estimate the effect of these electronic instabilities.

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Spectroscopic signatures of many-body correlations in magic angle twisted bilayer graphene

Yazdani, A.[1]

[1] ***Princeton University***

The discovery of superconducting and insulating states in magic angle twisted bilayer graphene (MATBG) has ignited considerable interest in understanding the nature of electronic interactions in this chemically pristine material system. The phenomenological similarity of the MATBG transport properties as a function of doping with those of the high-$T_c$cuprates and other unconventional superconductors suggests the possibility that MATBG may be a highly interacting system. However, there have not been any direct experimental evidence for strong many-body correlations in MATBG. I will describe experiments provide such evidence from high-resolution spectroscopic measurements, as a function of carrier density, with a scanning tunneling microscopy (STM). We find MATBG to display unusual spectroscopic characteristics that can be attributed to electron-electron interactions over a wide range of doping, including when superconductivity emerges in this system. We show that our measurements cannot be explained with a mean-field approach for modeling electron-electron interaction in MATBG. The breakdown of a mean-field approach for understanding the properties of other correlated superconductors, such as cuprates, has long inspired the study of highly correlated Hubbard model[3]. We show that a phenomenological extended Hubbard model cluster calculation, motivated by the nearly localized nature of the relevant electronic states of MATBG produces spectroscopic features similar to those we observe experimentally. Our findings demonstrate the critical role of many-body correlations in understanding the properties of MATBG.

Reference: Y. Xie et al. Nature 572, 101-105 (2019)

Topology and perfect metal in trilayer moiré graphene

Christophe Mora[1]

[1]*Laboratoire Matériaux et Phénomènes Quantiques (MPQ), Université Paris Diderot*

The past decade has witnessed remarkable experimental achievements in the study of two-dimensional materials such as graphene, graphene-like compounds or transition metal dichalcogenide (TMD) with the long-term goal of tailoring arbitrary heterostructures with desired properties. Stacking monolayers of graphene with a small twist angle forming moiré patterns has been demonstrated to dramatically change the band structure, generating gaps and band flattening in a controllable manner, forming in certain cases topological phases of matter as well as strongly correlated phases.
We discuss the electronic structure of a twisted multilayer graphene system forming a moiré pattern, focussing on small twist angles separating the graphene sheets. Extending beyond the bilayer case, we show that, when the ratio of the consecutive twist angles is rational, a periodicity emerges in quasimomentum space with moiré Bloch bands even when the system does not exhibit a crystalline lattice structure in real space. For a trilayer geometry, we identify one-dimensional flat bands that are relevant for the emergence of strong many-body effects.
Performing a symmetry analysis of the band model for trilayer, we prove that the system is a perfect metal in the sense that it is gapless at all energies. This striking result originates from the three Dirac cones which can only gap in pairs and produce bands with an infinite connectivity. The absence of gaps that we predict hold as long the combined C2zT symmetry is not broken.
More details : Flat bands and perfect metal in trilayer moiré graphene, C. Mora, N. Regnault, B. A. Bernevig, Phys. Rev. Lett. 123, 026402 (2019)

Internal screening and dielectric engineering in magic-angle twisted bilayer graphene

J.M. Pizarro[1,2], M. Rösner[3], R, Thomale[3], R. Valentí[4] and T.O. Wehling[1,2]

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[2] *Bremen Center for Computational Material Sciences, University of Bremen, Am Fallturm 1a, 28359 Bremen, Germany*

[3] *Institute for Molecules and Materials, Radbound University, NL-6525 AJ Nijmegen, The Netherlands*
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Magic-angle twisted bilayer graphene (MA-tBLG) has appeared [1] as a tunable testing ground to investigate the conspiracy of electronic interactions, band structure, and lattice degrees of freedom to yield exotic quantum many-body ground states in a two-dimensional Dirac material framework. While the impact of external parameters such as doping or magnetic field can be conveniently modified and analyzed, the all-surface nature of the quasi-2D electron gas combined with its

intricate internal properties pose a challenging task to characterize the quintessential nature of the different insulating and superconducting states found in experiments. We analyze [2] the interplay of internal screening and dielectric environment on the intrinsic electronic interaction profile of MA-tBLG. We find that interlayer coupling generically enhances the internal screening. The influence of the dielectric environment on the effective interaction strength depends decisively on the electronic state of MA-tBLG. Thus, we propose the experimental tailoring of the dielectric environment, e.g. by varying the capping layer composition and thickness, as a promising pursuit to provide further evidence for resolving the hidden nature of the quantum many-body states in MA-tBLG.

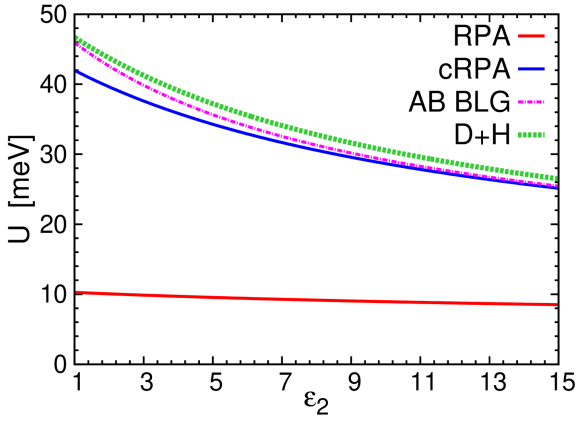

Figure 1: Dielectric engineering of the Hubbard interaction U in magic-angle twisted bilayer graphene encapsulated in a dielectric substrate and capping layer ε_2.

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Book of Abstracts: invited and contributed talks

Friday September 27th

Anomalous transport and quenched nematic criticality in $FeSe_{1-x}S_x$

Coldea A,[1]

[1] *Oxford University*

In this talk I will discuss magnetotransport studies in high magnetic field and quantum oscillations in FeSeS tuned either by chemical and applied pressure. I will discuss the electronic changes across the nematic phase transition and the power laws in resistivity across the nematic phase transition. Our results suggest that in the proximity of the nematic end point, the effective masses do not show divergent behaviour due to the quenching of nematic fluctuations by the interaction with the lattice. This effect also changes the power law in resistivity.

Effective Hall number across the strange metal regime of hole-doped cuprates

Hussey NE[1], Putzke C[2], Benhabib S[3], Tabis W[3], Ayres J[2], Wang Z[4], Lu J[1], Kondo T[5], Takeuchi T[6], Cooper JR[7], Carrington A[2]

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[2]*H.H. Wills Physics Laboratory, University of Bristol, Bristol, United Kingdom*
[3]*Laboratoire National des Champs Magnétiques Intenses (LNCMI-EMFL),Toulouse, France*
[4]*Hochfeld-Magnetlabor Dresden (HLD-EMFL), HZDR, Dresden Germany*
[5]*Institute for Solid State Physics, University of Tokyo, Kashiwa, Japan*
[6]*Toyota Technological Institute, Nagoya, Japan*
[7]*Department of Physics, University of Cambridge, Cambridge, United Kingdom*

Within conventional transport theory, the Hall number in the low temperature, high field limit $n_H(0)$ is simply related to the number of charge carriers and so its evolution with doping gives crucial information about the nature of the charge transport. Here we report a study of the high-field Hall coefficient of the single layer cuprates $Tl_2Ba_2CuO_{6+d}$ and La/Pb-doped $Bi_2Sr_2CuO_{6+d}$ across the so-called strange metal regime. We find that the hole concentration inferred from $n_H(0)$ increases smoothly from p to 1 + p, where p is the number of holes doped into the parent insulating state, over a wide range of the overdoped part of the phase diagram. Surprisingly, this evolution continues beyond the critical hole doping p* at which the normal state pseudogap closes. Indeed the evolution of $n_H(0)$ seems to correlate with the emergence of the anomalous linear-in-T term in the longitudinal resistivity rather than the appearance of a pseudogap and reveals a new property of the strange metal regime.

Linear in T and linear in |H| resistivity in cuprates, Heavy Fermions and Fe-based compounds.

Varma, C.[1]

[1] *Visiting Scientist, University of California, Berkeley.*

I will use the recently obtained T log T specific heat in the cuprates and the earlier such data in a heavy-fermion, both near quantum criticality, to extract parameters which are shown to be related to the measured single-particle relaxation rate, resistivity and density correlations, as given by the theory of the criticality of the quantum xy model. The change of resistivity to linear in |H| for \mu_B |H| >> k_BT is shown to be a direct proof of the topological nature of excitations responsible for the transport. A remarkable result that comes from the Monte-carlo and RG solution of the problem is a parameter range of |H| in which the correlation functions become periodic in time.

Universal *T*-linear Resistivity and Planckian Dissipation in Overdoped Cuprates

Cyril Proust[1]

[1]*Laboratoire National des Champs Magnétiques Intenses, Toulouse, France*

The perfectly linear temperature dependence of the electrical resistivity observed as T → 0 in a variety of metals close to a quantum critical point (QCP) is a major puzzle of condensed matter physics [1-3]. In cuprates, a T-linear resistivity as T → 0 has been observed in few families once superconductivity is suppressed by a magnetic field. On the electron-doped side, T-linear resistivity is seen just above the QCP where AF order ends [4]. On the hole-doped side, however, the doping values where T-linear is observed are very far from the QCP where long-range AF order ends. Instead, these values are close

to the critical doping where the pseudogap phase ends [5]. Several questions must be answered. Is T-linear resistivity generic in cuprates? Is there a common mechanism linking cuprates to the other metals where r ~ T as T → 0? We measured the low-temperature resistivity of the bi-layer cuprate $Bi_2Sr_2CaCu_2O_{8+d}$ and found that it exhibits a T-linear dependence with the same slope as in the other hole-doped cuprates. It has been proposed that T-linear resistivity may be associated with the scattering rate 1 / t reaching the Planckian limit, i.e. $\hbar / \tau = k_B T$ [6, 7]. We show that the Planckian limit is obeyed in all cuprates where a pure T-linear resistivity has so far been observed.

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Dynamical Charge Density Waves pervading the phase diagram of High-T_c Superconducting Cuprates

M. Grilli[1]

[1]*Dipartimento di Fisica, Università di Roma `Sapienza', 00185, Rome, Italy*

According to an old proposal [1] recently revised and extended [2], charge density waves (CDW) arise below the pseudogap crossover temperature T* from a quantum critical point around optimal doping. Due to the near two-dimensionality of the CuO_2 planes, disorder, and competition with superconductivity, the nearly critical CDW usually stay dynamical without forming a long-ranged state. The unexpected occurrence of CDW fluctuations even in the overdoped region of Bi2201 cuprates [3] confirms that CDW in cuprates are a pervasive effect in these systems.

Recent Resonant X-ray Scattering experiments [4] provide clear evidence that strong, very short-ranged dynamical charge density fluctuations (CDF) with characteristic wavevector similar to that of CDW are present up to very large T above T* and in the overdoped region of Nd-123 samples and coexist with CDW below T*. This will stimulate a revision of the current understanding of the charge fluctuation phenomenon in cuprates since these CDF could in fact provide a possible mechanism for the Marginal Fermi Liquid behavior of these systems in the normal state [5].

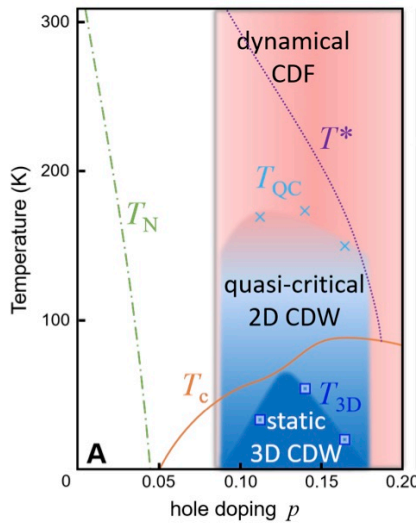

Fig. 1: (From [4]) Summary NBCO phase diagram from RXS experiments. Increasing blueish

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Interplay between CDW and superconducting fluctuations: a new perspective

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The phase diagram of underdoped cuprates is extremely rich and complex. In addition to a transition from an antiferromagnetic insulator at half-doping to a strange metal at optimal doping, and the opening of a pseudogap in the density of states, the normal state is also the location for charge ordering (CO) and Fermi surface reconstruction. By analyzing $La_{1-x}Sr_xCuO_4$ thin films resistivity under high pulsed magnetic field for various dopings, we extract a systematic (H,T) phase diagram

and we discuss the interplay between CO and superconductivity. In particular we relate our findings to a theoretical model [1,2], which enables to demonstrate that disorder can induce a charge-density-wave (CDW) to become superconducting. This paradoxical effect occurs close to the phase boundary between CDW and SC and is analogous to the occurrence of supersolid effects in ^{4}He. It originates from the topological stabilization of filamentary superconductivity at the interfaces of different CDW domains. By comparing experimental and theoretical phase diagrams we show that the previously observed two-step phase transition in under-doped films [3] is related to the interplay between superconducting fluctuations and dynamic CDW [2].

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From Mott to Not: Phenomenology of the Overdoped Cuprate Superconducting State

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New experimental data on superfluid density and terahertz conductivity of overdoped LSCO have exhibited behavior incompatible with a clean BCS superconductor [1]. Many of the properties observed are however compatible with “dirty d-wave theory” assuming weak scattering by dopant atoms [2,3]. Here we test these ideas by comparing to specific heat and thermal conductivity data on LSCO, showing that the theory works extremely well across the overdoped region for similar disorder parameters. We then study the same properties in another overdoped cuprate, Tl-2201, thought to be quite clean since it exhibits quantum oscillations, low residual resistivities and small superconducting state Sommerfeld coefficients. Our results are consistent with the Tl-2201 system being ~3 times cleaner due in part to the dopant atoms being located further from the CuO2 plane[3]. We conclude that overdoped cuprates can be described semiquantitatively by dirty d-wave theory, subject to significant Fermi liquid renormalizations, without introducing physics beyond the Landau-BCS paradigm.

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Synchrotron x-ray studies of the Charge Density Wave order

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The nature of the charge-density wave (CDW) order is currently one of the most intensively discussed topics in the field of high-T_c cuprates. The doping dependence of the two-dimensional (2D) CDW wavevector in $HgBa_2CuO_{4+d}$ (Hg1201) provides strong evidence that these correlations, assuming that they are bi-directional, are responsible for the Fermi-surface reconstruction [1,2]. In contrast, some measurements in $YBa_2Cu_3O_{6+d}$ (YBCO) indicate that the 2D CDW order is consistent with a local unidirectional "stripe" order [3], while long-range order that causes reconstruction is due to an additional three-dimensional (3D) charge order triggered by external magnetic fields [4]. We will discuss resonant X-ray scattering measurements performed under uniaxial pressure and X-ray absorption spectroscopy in pulsed fields in Hg1201, YBCO and Nd_{2-x} Ce_xCuO_4. The data support the bi-directional character of the 2D CDW correlations. The emergence of the 3D order in YBCO might be specific to this compound.

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Entangled preformed Cooper and Excitonic pairs in cuprate superconductors

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Despite having been discovered nearly 30 years ago, cuprate superconductors still offer new experimental and theoretical developments. At the center of the mystery lie the pseudogap phase from which a superconducting phase emerges. However the pseudogap is also the host of multiple other orders, the question is then to identify which contribution is the most relevant. One of the recent focus has been on the observation of a modulated superconducting order, or Pair Density Wave (PDW), in the halo of superconducting vortices[1] which has been proposed to give rise to the pseudogap in multiple approaches (e.g [2]). There is however a recent Raman spectroscopy study that shows that the superconducting order is very close energetically to the Charge Density Wave (CDW) that appears in the pseudogap phase[3]. We present here a new idea to describe the pseudogap as a phase of entangled particle-particle (Cooper) and modulated particle-hole (Excitonic) pairs[4]. These pairs get

entangled at a high temperature associated with the pseudogap while giving rise to the known superconducting and CDW orders respectively at a lower temperature. The entanglement can be obtained as a result of a particular Higgs mechanism or as a result of the fractionalization of a PDW order. It is thus able to link multiple experimental observations and we present here connections with results from Angle-Resolved Photoemission Spectroscopy, Raman spectroscopy and Scanning Tunneling Microscopy.

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Disorder raises the critical temperature of a cuprate superconductor

M. Leroux[1,7], V. Mishra[1,8], J. P.C. Ruff[2], H. Claus[1], M. P. Smylie[1,9], C. Opagiste[3], P. Rodière[3], A. Kayani[4], G. D. Gu[5], J. M. Tranquada[5], W.-K. Kwok[1], Z. Islam[6], and U Welp[1]

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With the discovery of charge density waves (CDW) in most members of the cuprate high temperature superconductors, the interplay between superconductivity and CDW has become a key point in the debate on the origin of high temperature superconductivity. Some experiments in cuprates point toward a CDW state competing with superconductivity, but others raise the possibility of a CDW-superconductivity intertwined order, or more elusive pair-density wave (PDW). Here we have used

proton irradiation to induce disorder in crystals of La1.875Ba0.125CuO4 and observed a striking 50% increase of Tc accompanied by a suppression of the CDW. This is in sharp contrast with the behavior expected of a d-wave superconductor for which both magnetic and non-magnetic defects should suppress Tc. Our results thus make an unambiguous case for the strong detrimental effect of the CDW on bulk superconductivity in La1.875Ba0.125CuO4. Using tunnel diode oscillator (TDO) measurements, we find indications for potential dynamic layer decoupling in a PDW phase. Our results establish irradiation-induced disorder as a particularly relevant tuning parameter for the many families of superconductors with coexisting density waves, which we demonstrate on superconductors such as the dichalcogenides and Lu5Ir4Si10. [1]

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Metallic and insulating stripes and their relation with superconductivity in the doped Hubbard model

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The dualism between superconductivity and charge/spin modulations (the so-called stripes) dominates the phase diagram of many strongly-correlated systems, as the Hubbard model. Here, we investigate this antagonism within a variational Monte Carlo approach that is based upon Jastrow-Slater wave functions, including backflow correlations. We find that stripe order with periodicity λ=8 in the charge and 2λ=16 in the spin can be stabilized at doping δ=1/8, in agreement with Ref.[1]. Here, there are no sizable superconducting correlations and the ground state has an insulating character. A similar situation, with λ=6 appears at δ=1/6. Instead, for smaller values of dopings, stripes can be still stabilized, but they are weakly metallic at δ=1/12 and metallic with strong superconducting correlations at δ=1/10, as well as for intermediate (incommensurate) dopings. Remarkably, we observe that spin modulation plays a major role in stripe formation, since it is crucial to obtain a stable striped state upon optimization [2].

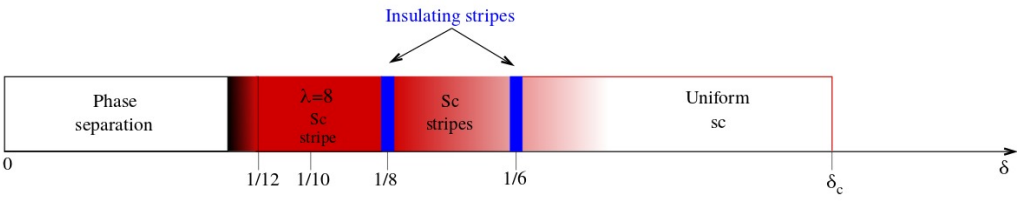

Figure 1: Schematic phase diagram of the doped repulsive Hubbard model at *U/t=8* on a 6-leg ladder. The graduated shading indicates the progressive weakening of the stripe order.

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Tuning superconductivity in atomically thin materials with space charge doping

Johan Biscaras[1], *Fang* Wang[1], *Edoardo* Sterpetti[1], *Andreas* Erb[2], *Abhay* Shukla[1]

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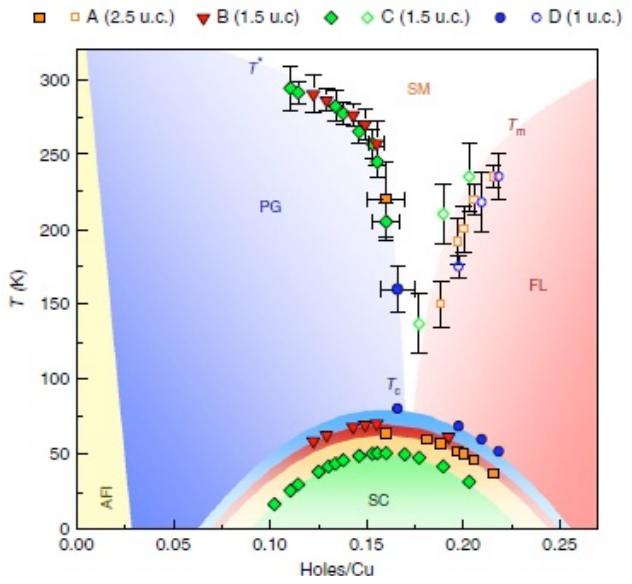
[2]***Walther Meissner Institut fur Tieftemperaturforschung, Bayerische Akademie der Wissenschaften, Walther-Meissnerstr. 8, 85748 Garching, Germany***

We have developed a new electrostatic doping technique called “space charge doping” capable of inducing ultra high carrier densities in 2D electronic systems. It is ideally suited to dope ultra-thin layered materials and explore their phase diagram as a function of electronic density, without chemical doping.

We will present the technique and show its application to few unit-cell thick Bi-2212 a high temperature superconductor cuprate. Using space charge doping we established the phase diagram of Bi-2212, as seen by transport measurements, in a large doping range around the optimal doping while taking disorder as a further parameter. At lower doping, we induce a Superconductor - Insulator Transition whose critical behaviour will be discussed.



Pseudo Landau levels, non-local exchange and quantum anomalous Hall effect in twisted bi-layer graphene systems

Dai, Xi[1,2]

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We propose that the electronic structure of twisted bilayer graphene (TBG) can be understood as Dirac fermions coupled with opposite pseudomagnetic fields generated by the moiré pattern. The two low-energy flat bands from each monolayer valley originate from the two zeroth pseudo Landau levels of Dirac fermions under such opposite effective magnetic fields, which have opposite sublattice polarizations and carry opposite Chern numbers +1/-1, giving rise to helical edge states in the gaps below and above the low-energy bulk bands near the first magic angle. With the presence of long range Coulomb interaction, the non-local valley exchange process will lead to two types of possible spontaneous symmetry breaking phases, the first one breaks the valley U(1) symmetry and leads to featureless insulator phase and the second one breaks the time reversal symmetry in the orbital sector and leads to non-zero Chern number, which is consistent with the recent experimental discovery of the quantum anomalous Hall effect in these systems.

Book of Abstracts: invited and contributed talks

Saturday September 28th

High-T_c Superconductivity in Dense Hydrogen Systems

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Recent theoretical and experimental investigations of hydrogen-rich materials at megabar (>100 GPa) pressures are opening a new era of study of high T_c superconductivity in the vicinity of room temperature. We predicted and experimentally confirmed the existence of a new class of such materials, superhydrides (MH_x, with $x > 6$), and developed techniques for syntheses and characterization of their structural and transport properties at megabar pressures. Superhydrides in the La-H system superconduct at temperatures from 150 K to 260 K at pressures near 200 GPa [1]. The results for the highest T_c phase, LaH_{10}, were subsequently confirmed [2], and a growing number of other superconducting superhydride phases are now being documented experimentally by other groups. The superconductivity in these systems is consistent with conventional phonon-mediated superconductivity, but with unconventionally strong quantum and anharmonic character. There are prospects for observing T_c's well above room temperature in more complex hydrogen-rich systems as well as in pure atomic metallic hydrogen.

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High-Tc Superconductivity at High Pressures

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In less than five years, the discovery of high-temperature superconductivity in two high-pressure hydrides, SH3 and LaH10, has revolutionized the field of superconductivity, setting a record for

Tc to almost room temperature (260 K), and opening a new route to search for new superconductors which strongly relies on computational methods for crystal structure prediction and superconductivity.
The two recent reports of metallisation in hydrogen, and superconductivity in yttrium hexahydride, further raise the hope that room-temperature superconductivity may be achieved in the near future.
In my contribution, I will review the current theoretical understanding of the field of superconductivity in high-pressure hydrides and propose possible strategies to obtain conventional superconductors with improved superconducting properties. [1]

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Observation of the transition to metal hydrogen: a stepping stone towards disclosing novel quantum many-body effects.

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Understanding how and when molecular solid hydrogen may transform into a metal has stimulated many theoretical works since the 30's and it is still an open question. On the other hand, the quest for metal hydrogen has pushed major developments of modern experimental high pressure physics, yet the various claims of its observation have remained unconfirmed.
Recently, we observed and characterized the transition to metal hydrogen near 425 GPa at 80 K [1]. From previous measurements of the change of the direct bandgap in the visible, showing a linear decrease up to 300 GPa, closure of the direct bandgap, hence the insulator-metal transition, was expected to occur about 460 GPa [2]. The most advanced theoretical calculations obtained also the stability of metal hydrogen in the 400 GPa – 500 GPa pressure range[3, 4].
In this talk, we will present our experimental strategy, namely: 1) Demonstrate the possibility to generate pressures well over 400 GPa since this pressure range is the limit of the conventional Diamond Anvil Cell (DAC); 2) Exhibit a reliable non-intrusive signature of the insulator-metal phase transition, i.e total IR absorption; 3) Record combined infrared, Raman and visible observation measurements to disclose the physics at stake at the insulator-metal transition. A first order transition from a molecular insulator to a protons paired metal is suggested.
Finally, we will discuss some future experimental developments that could be implemented to reveal the quantum-many body properties of this intriguing system, such as a room temperature superconductivity.

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Crystal prediction in dense hydrogen systems: the crucial role of quantum ionic effects

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The discovery of superconductivity at 200 K in the H_2S system at large pressures shows that H-rich compounds can be high-Tc superconductors. The synthesis of LaH_{10} with Tc=250 K, together with the possible one of yttrium and thorium hydrides, place these materials at the verge of reaching room-temperature superconductivity. Many of these discoveries rely to some extent on material by design calculations that, often, neglect quantum ionic effects. However these are known to be extremely large in H-based systems.

Here I will present calculations on H_3S and LaH_{10} and I will show that nuclear quantum effect reshape the high pressure phase diagram of these materials. Furthermore, quantum effects reveal crucial to sustain solids with extraordinary electron-phonon interaction, that otherwise could be destabilized, demonstrating that these systems are Quantum Crystals.

Metallicity driven by thermal amplification of the carrier mass in SrTiO3

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Strontium titanate is a wide-gap semiconductor avoiding a ferroelectric instability thanks to quantum fluctuations. This proximity leads to strong screening of static Coulomb interaction and paves the way for the emergence of a very dilute metal with extremely mobile carriers at liquid-helium temperature

[1]. Upon warming, mobility decreases by several orders of magnitude. Yet, metallicity persists above room temperature even when the apparent mean-free-path (deduced from the magnitude of the resistivity and the effective mass obtained from quantum oscillations) falls below the electron wavelength [2]. Here we will present new resistivity and thermoelectrical datas extending up to 1000K to follow the fate of this enigmatic metallicity at high temperature [3]. We will show that it is a result of a significant increase of the mass carrier with temperature. We will discuss this high temperature mass enhancement at the light of the temperature dependence of the phonon spectrum as measured by inelastic neutron scattering.

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Unconventional electronic transport from the scattering off slow bosons

Simone Fratini[1]

[1] ***Institut Néèl, CNRS, Grenoble***

The presence of thermally excited low energy bosons causes the electronic resistivity to vary linearly with temperature, as observed in normal metals at high temperature. This simple picture, which follows from the equipartition principle in the weak scattering regime, is modified when multiple scattering processes are considered. This is required when the energetic fluctuations associated to the bosonic field are large on the scale of the electronic kinetic energy: slow bosons then behave as quasi-static scatterers, enabling quantum localization processes whose principal signatures are the emergence of displaced Drude peaks and the breakdown of the Mott-Ioffe-Regel limit. In this talk I shall review the theory of transient localization, that was devised to describe such anomalous transport regime as resulting from the abundance of slow inter-molecular phonons in organic semiconductors, and speculate on its possible application to correlated systems and its relation to Planckian dissipation.

Book of Abstracts: posters

Entanglement properties in quantum phases of the asymmetric two-leg Hubbard ladder

Anas Abdelwahab[1] and Eric Jeckelmann[1]

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We investigate entanglement properties of an asymmetric two-leg Hubbard ladder that consists of one Hubbard leg and one tight-binding leg[1][2]. We use the density matrix renormalization group method to study the von Neumann entropy, central charge, Schmidt gap and entanglement spectrum for different quantum phases that appear by varying the inter-leg hopping term. We can distinguish the gapless and the correlated band insulating phases[1][2] using the entanglement properties in the ground state. The differences in entanglement properties between the Kondo-Mott and the spin-gaped Mott insulating phases[1][2] are less clear.

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Hydrostatic vs. Chemical pressure effects on the MIT and on the nematic antiferromagnetic order of $BaCoS_2$

HaneenAbushammala[1], Pierre Toulemonde[2], Yannick Klein[1], Andrea Gauzzi[1]

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The quasi-2D $BaCoS_2$ (BCS) system displays an unusual gapless Mott state concomitant with a nematic antiferromagnetic (AFM) ordering at T_N=305 K of the Co^{2+} ions in the square-lattice [1]. Either electron doping, achieved by a partial Co/Ni substitution [2], or hydrostatic pressure [3] drives the system into a paramagnetic and Fermi Liquid (FL) metallic phase. Interestingly, this metal-insulator transition (MIT) is not accompanied by any significant structural distortion, which offers ideal conditions to investigate the FL to non-FL crossover in a model square-lattice system in the regime of moderate electronic correlations typical of sulfides.

One open question regarding the microscopic origin of the MIT is the interplay between AFM order and Mott state. In order to investigate this issue, we have studied the effects of chemical pressure on the AFM order by partially substituting Ba for Sr. Contrary to the case of hydrostatic pressure, we find

that chemical pressure significantly reduces T_N down to 240 K for a substitution level of 8 at% only, corresponding to an effective pressure of 0.3 GPa. This result is explained by a reduction of the superexchange interaction energy, J, by chemical pressure. Further studies are required to investigate the changes in the electronic structure responsible for this reduction and whether higher substitution levels may fully suppress the AFM order and stabilize a FL phase.

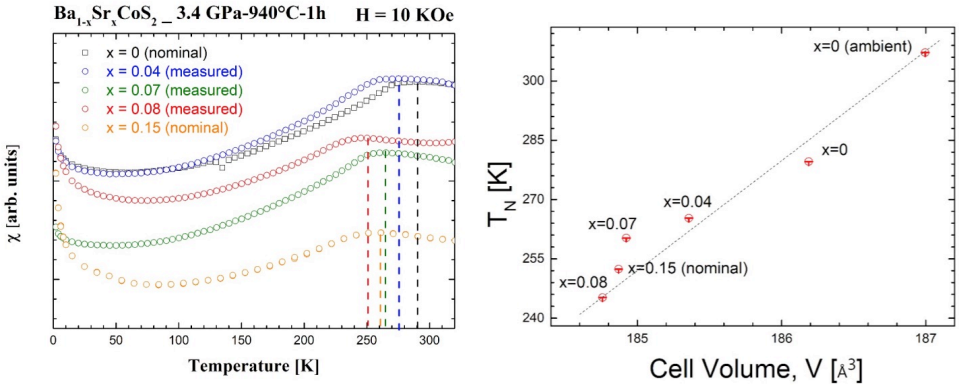

Figure 1: On the left, the susceptibility measurement of x-components as a function of temperature. On the right, the T_N of x-components as a function of cell volume.

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Non-equilibrium Kondo effect: connecting an impurity to chains in the Luttinger liquid phase

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[2] *International Institute of Physics and Department of Theoretical and Experimental Physics, Federal University of Rio Grande do Norte, Natal, RN, Brazil*

We study the effects of electronic interactions on the formation of the Kondo screening cloud within time dependent density matrix renormalization group. We follow the non-equilibrium dynamics after a quench that connects a magnetic impurity to interacting chains, which are in the Luttinger liquid phase of the Hubbard model at quarter-filling. According to our results, antiferromagnetic correlations between the impurity and the conducting electrons (and thus the Kondo cloud) form faster for larger interaction U in the chains and smaller interaction U_d at the impurity. The bipartite entanglement entropy (EE), by its turn, shows a stronger dependence on U_d than on U. Changes in the charge occupation and in the local spin follow effective light cones, defined by different velocities, in accordance with spin-charge separation of one-dimensional Hubbard model; in the case of EE, light cones are defined by the fastest velocity, corresponding to charge excitations.

Emergent superconductivity upon disordering a charge density wave ground state

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We explore the interplay of a charge density wave (CDW) order and s-wave superconductivity in a disordered system [1]. Recent experiments on 1*T*-$TiSe_2$, where the pristine sample has a commensurate CDW order and the superconductivity appears upon copper intercalation, motivates our study. Starting with an extended Hubbard model, with parameters that yield a CDW ground state within Hartree-Fock-Bogoliubov formalism in pure systems, we show that the addition of disorder quickly wipes out the global charge order by disrupting periodic modulation of density at some (low) strength of disorder. Along with this, the subdominant superconducting order emerges in regions that spatially anticorrelate with islands of strong local CDW order. The short-range density modulations, however, continue to persist and show discernible effects up to a substantial disorder strength. The local CDW puddles reduce in size with increasing disorder, and they finally lose their relevance in affecting the properties of the system. Implications of our results for the experimental phase diagram of transition-metal-dichalcogenides will also be discussed.

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Coexistent solutions and first-order transition between two metals in the 2-D Hubbard model with Cellular and DCA-DMFT

Lorenzo Fratino[1,2], Hiroshi Shinaoka[3], Yusuke Nomura [4], Luca de' Medici[2]

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We explore the phase diagram of the 2-dimensional Hubbard model, believed to capture the physics of cuprates, in order to investigate the nature of the Mott transition and its fate as function of doping using Dynamical Cluster Approximation Dynamical Mean Field Theory (DCA DMFT) [1] [2] solved with continuous time quantum Montecarlo (CTQMC) [3]. The nature of the insulating to metal transition at half filling has been tested in order to verify the existence of meta-stable coexisting solutions at finite temperature, as never showed with this methodology in contrast with other methods, e.g. [4], and [5]. In particular, we then focus on the pseudogap-phase-to-correlated-metal transition [6] and we confirmed an existence of meta-stable coexisting solutions at finite temperature and finite doping as found in previous work with different methodology,e.g. [4], [7].

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Impact of non-local exchange on Iron Pnictides

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Ten years after their discovery, the physics of iron-based superconductors (IBSC) has yet to be clarified, and a unified understanding of their behaviour is far from being reached. Even though the major role played by local correlations has been widely assessed, low-energy models relying exclusively on them are not able to reproduce some fundamental properties, most notably the size of electron and hole pockets of the Fermi surface [1,2]. In this regard, we study the effect of non-local exchange in the presence of strong local correlations within the IBSC 122-family, by means of Slave-Spin@Density-Functional Theory simulations. Non-local exchange is treated at the DFT level via the screened hybrid functional HSE06, whereas local Hubbard- and Hund-type interactions are accounted for within the Slave-Spin method. Particular attention will be given to the impact of non-local interactions on the Fermi surface, via a thorough comparison with the available experimental data for different electron doping and degree of correlation.

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Probing Topological edge states by measuring transport through an interacting magnetic impurity

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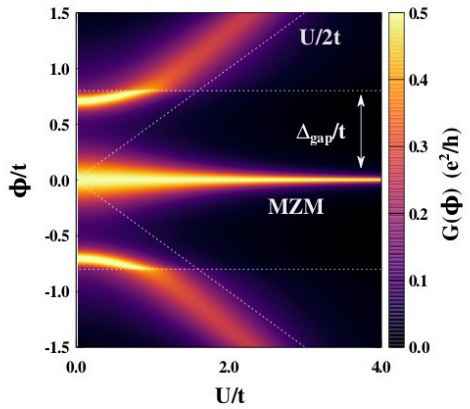
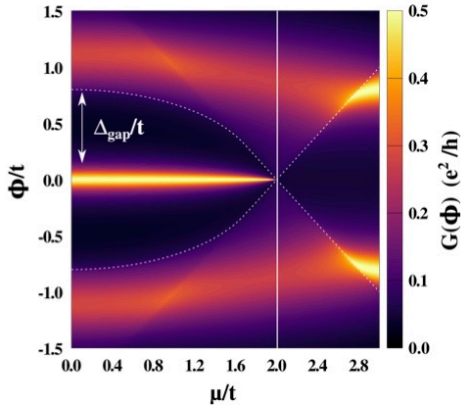
Motivated by recent experiments [1,2] we consider transport across an interacting magnetic impurity coupled to the Majorana zero mode (MZM) observed at the boundary of a topological superconductor. In the presence of a finite tunneling amplitude we observe hybridization of the MZM with the quantum dot, which is manifested by a fractional zero-bias anomaly in the conductance $G_0=e^2/2h$ measured on the metallic contacts [3].
The low-energy feature in the conductance drops abruptly by crossing the transition line from the topological to the non-topological superconductive phase. Differently from the in-gap Yu- Shiba-Rosinov bound states, which are strongly affected by the on-site impurity Coulomb repulsion, we show that a the MZM signature in the conductance is robust and persists even at large values of the interaction. To perform a complete characterization of the junction we compute the shot-noise and the Fano factor.
Despite being interacting the model is exactly solvable by means of the Z_2 slave-spin mapping [4], which allows to have an exact characterization of the transport properties of the junction.



Influence of the interaction U/t on the conductance $G(\phi)$. Horizontal dashed line show the width of the bulk superconductive gap Δ_{gap}. The on-site repulsion U competes with the coupling to the Majorana mode γ_1 by shrinking the zero-bias conductance.



Evolution of the conductance as a function of μ/t. In correspondence of the topological transition μ/t=2, that is outlined by the white vertical line, the zero-bias anomaly $G_0=e^2/2h$ disappears. Dashed white line shows the superconductive gap measured on the boundary site of the semi-infinite Kitaev chain.

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Departure from the Wiedemann-Franz Law in WP_2 Driven by Mismatch in T-square Resistivity Prefactors

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We present a study of the electrical and thermal conductivities of the semimetal WP_2 in the T = 2K - 40K temperature range. At low-temperature, the Wiedemann-Franz law (WF law) holds, but upon warming, a downward deviation from the WF law is observed. In the case of WP_2 [1], the difference reaches an exceptionally large value compared to what has been previously reported in other metals [2]. We identify small-angle electron-electron scattering as the origin of this departure [3]. We were further able to quantify the mismatch in the frequency of inter-electronic collisions which conserve momentum (i.e. electric current) but degrade energy (as in the case of normal-state liquid ^{3}He). This sets a narrow temperature window between the ballistic and diffusive regimes where the hierarchy of scattering times corresponds to the hydrodynamic requirements for charge carriers [4].

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Pulsed field measurements capabilities at the LNCMI Toulouse: torque magnetometry, resistivity and NMR

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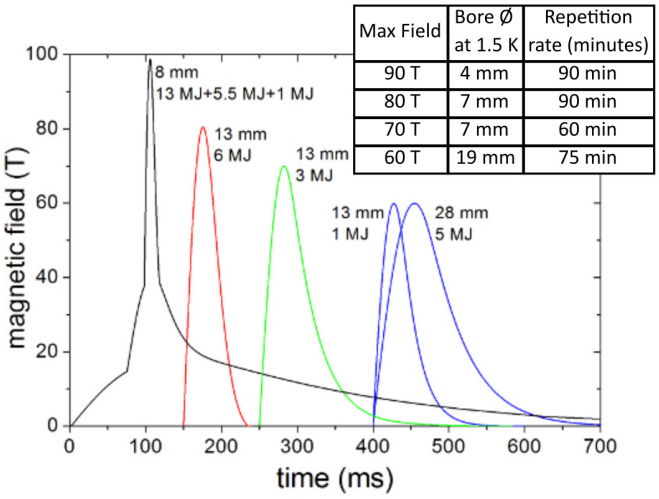
The Toulouse National High Magnetic Field Laboratory (LNCMI-T) is a user facility for experiments in pulsed magnetic fields. The LNCMI-T has already provided more than 100 shots at 90 T to its international user base, with pulses duration of 100s of milliseconds (Fig.1). Coils for 80, 70 or 60 T (and any field below) are also available. In addition, a single turn magnet facility provides access to fields up to 250 T at the microsecond scale. Standard experimental techniques available to users include electrical transport, torque magnetometry, NMR, ultrasound and optical/IR spectroscopy. The LNCMI-T is located in Toulouse in southwestern France and it is one of the 4 facilities of the European Magnetic Field Laboratory (EMFL), with other sites in Nijmegen, Grenoble and Dresden. Magnet time is allocated to external researchers after submission of a proposal and review by an international selection committee. Deadlines twice yearly: Nov. 15th/May 15th
https://emfl.eu/apply-for-magnet-time/



Max Field	Bore Ø at 1.5 K	Repetition rate (minutes)
90 T	4 mm	90 min
80 T	7 mm	90 min
70 T	7 mm	60 min
60 T	19 mm	75 min

Figure 1: Summary of LNCMI-T pulsed field capabilities

Phonon thermal Hall effect in strontium titanate

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It has been known for more than a decade that phonons can produce an off-diagonal thermal conductivity in presence of magnetic field[1]. Recent studies of thermal Hall conductivity, k_{xy}, in a variety of contexts, however, have assumed a negligibly small phonon contribution. We present a study of k_{xy} in quantum paraelectric $SrTiO_3$ and find that its peak value exceeds what has been reported in any other insulator, including those in which the signal has been qualified as 'giant'[2]. Remarkably, $k_{xy}(T)$ and $k(T)$ peak at the same temperature and the former decreases faster than the latter at both sides of the peak. This hitherto unreported behavior is also visible in the case of La_2CuO_4 and α-$RuCl_3$. We also studied $KTaO_3$ and found a small signal, indicating that a sizable $k_{xy}(T)$ is not a generic feature of quantum paraelectrics. Combined to other observations, this points to a crucial role played by antiferrodistortive domains in generating $k_{xy}(T)$ of this solid.

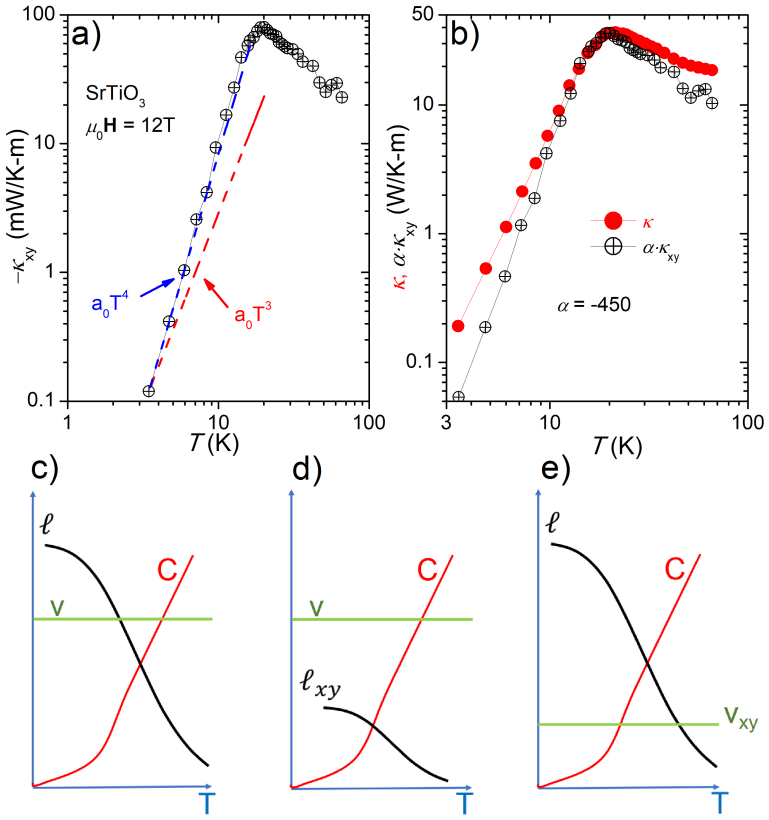

Figure 1: Thermal Hall conductivity and its correlation with longitudinal thermal conductivity. (a) The temperature dependence of κ_{xy} in presence of a magnetic field of 12T in $SrTiO_3$. (b) A comparison of the temperature dependence of longitudinal and transverse thermal conductivity, κ_{xy} has been multiplied by a factor α equal to -450. Both peak at the same temperature, but κ_{xy} falls faster at both sides of the peak. (c) Schematic sketch of the temperature dependence of specific heat, mean-free-path and velocity generating a peak in κ. Off-diagonal response may be caused by the skew scattering (transverse mean-free-path l_{xy} (d) or the off-diagonal velocity v_{xy} (e)).

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Impact of interfacial defect on electronic and transport properties at the FeRh/MgO/FeRh (001) MTJ from first-principles investigations

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Metal/oxide interface has raised a considerable interest due to its applications in spintronic devices. It plays critical roles in many applications including material science, microelectronic and chemical applications. As metal we choose FeRh equiatomic phase in the CsCl structure, which has paid attention in the last decade due to its fundamental properties of the first order phase transition. This transition is accompanied by a volume expansion of about 1% from the antiferromagnetic (AFM) to ferromagnetic (FM) phase [1]. The choice of the MgO as substrate is verified by its high chemical, thermal and mechanical stability, which allow it to be widely used as substrate for epitaxial growth.

In other hand, oxidation of ferromagnetic electrodes at the interface or oxygen vacancy could affect the electronic, magnetic and, thus, transport properties. Therefore, significant research efforts were devoted to the problem of oxygen layer formation at the Fe/MgO interface, and its influence on transport properties [2, 3]. In MTJs, the tunneling magnetoresistance effect (TMR) has been shown to be strongly affected by the presence of oxide or nonmagnetic metal layers at the interface [4].

By means of first-principles density functional theory (DFT) as implemented in the TRANSIESTA package [5] calculations, a theoretical study of the electronic structure and spin-dependent transport properties at the FeRh/MgO/FeRh (001) MTJ is reported. We analyzed the impact of interface oxidation and oxygen vacancy on the transport properties. The oxidation modifies crucially the electronic structure and the magnetic properties. Our results indicated that the oxygen vacancy at the FeRh/MgO interface increases the spin polarization at the Fermi level.

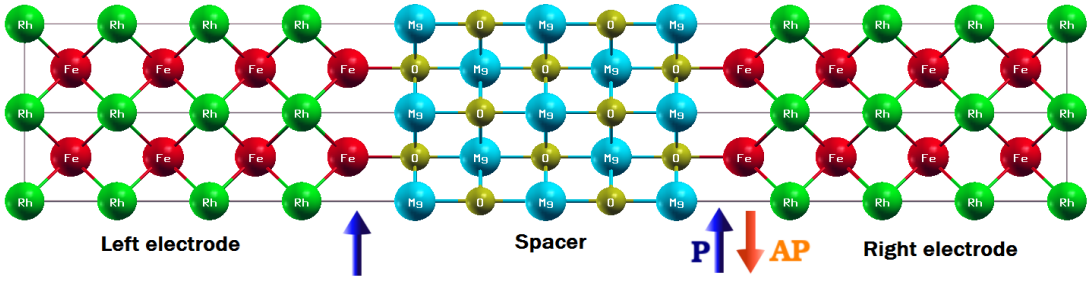

Figure 1: Schematic representation of the FeRh/MgO/FeRh (001) MTJ, P and AP are the parallel and antiparallel magnetic orientations of the two electrodes, respectively.

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Incipient loop current order in the under-doped cuprate superconductors

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Growing experimental evidence indicate discrete symmetry breaking like parity, time-reversal and C_4 lattice rotation in the pseudo-gap state of the under-doped copper-oxide based (cuprate) superconductors. The discrete symmetry breaking manifests a true phase transition to an ordered state. A detailed understanding of the nature of transition of these orders can answer various puzzles related to the nature of the transition at the pseudo-gap temperature T^*. In this work, we investigate the origin of time-reversal and parity symmetry breaking in the pseudo-gap state, considering bond-density wave (BDW) order and superconductivity (SC) as primary orders. We demonstrate how the fluctuations of the BDW and SC orders become important to the time-reversal and parity breaking in the pseudo-gap state.

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One to two-band superconductivity transition driven by gate voltage at an oxide interface

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The two dimension electron gases (2DEG) at the two band-insulator oxide interface LaAlO3/SrTiO3, first discovered in 2004 [1] have raise interest as it can host multiple electronic states including metallic, insulating or superconducting, and its properties are tuneable with a gate voltage [2][3].

In this context, we've probed the superfluid stiffness of the condensate at the LaAlO3/SrTiO3

interface, where SrTiO3 is oriented in the (110) direction, using resonant micro-wave measurement at mK temperature. Our work provides evidence of a transition from single to two-condensate superconductivity, driven by continuous and reversible electrostatic doping. We find that the superconductivity gap is suppressed as the second band is populated. Such behaviour is not expected in the Bardeen-Cooper-Schrieffer theory and can be explained using repulsive coupling between the condensate, characterized by an opposite sign in the order parameter. [4]

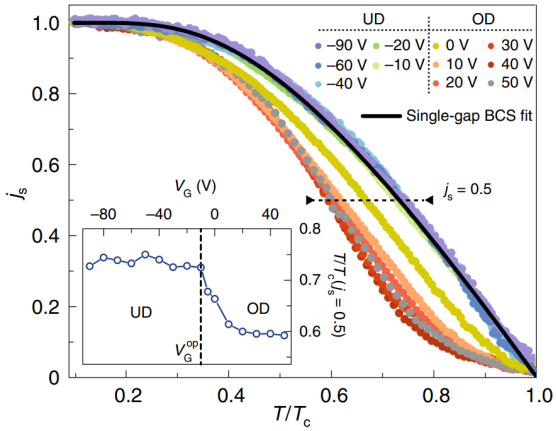

Figure : Normalized superfluid stiffness js as a function of the reduced temperature T/Tc for different gate voltages. In the under-doped (UD) regime, all the curves are superimposed and follow a single-gap BCS behavior (dashed line). In the over-doped (OD) regime, the temperature dependence of the js curves is strongly modified. Inset, reduced temperature T/Tc corresponding to js = 0.5 as a function of gate voltage. Whereas the values are constant in the UD regime, an abrupt decrease takes place at the Liftshitz transition.

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Metal-Insulator transitions in disordered correlated systems away from half-filling

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In this work we study strongly correlated electron systems in the presence of disorder. The interplay between interaction and disorder can be studied by considering the Anderson-Hubbard model [1]. To solve this model we use the Dynamical Mean-Field theory (DMFT) [2] together with the Typical-Medium Theory (TMT) methodology [3]. Our results show that there are three phases in the system in the doped case: a metal, a Mott insulator (MI), and an Anderson-Mott insulator (AMI). Within AMI, we observe a region where the average density of states around the Fermi level presents a power-law, V-shaped behavior (V-AMI). The phase AMI exists for large interaction and intermediate disorder; in this

case there are sites with double occupation and sites that are single occupied. V-AMI region appears for larger disorder, when some of the sites become empty. By changing the interaction, disorder, and doping, we explore for which sets of parameters the V-AMI is observed.

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Quantum well states for graphene spin-texture engineering

Vincent T.[1], Voloshina E.[2,3,5], Pons S.[1], Simon S.[4], Fonin M.[4], Wang K.[3], Paulus B.[3], Roditchev D.[1], Dedkov Y.[2,3,5] and Vlaic S.[1]

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The modification of graphene (Gr) band structure, in particular via induced spin-orbit coupling, is currently a great challenge for the scientific community with the final goal to achieve novel quantum phases and properties in Gr [1]. Here, we investigate the modification of the electronic structure of Gr on Ir(111) via intercalation of one monolayer Pd by means of angle-resolved photoelectron spectroscopy and density functional theory. We reveal that, for the Gr/Pd/Ir(111) intercalated system, a spin splitting of Gr π states higher than 200meV is present near the K_{Gr} point which arises from the hybridization of the Dirac cone with spin-polarized quantum well states of Pd on Ir(111). Our results demonstrate that the proposed approach on the tailoring of the dimensionality of heavy materials interfaced with a Gr layer might lead to induced giant spin-orbit splitting of the Gr valence band states, making such systems extremely appealing for Gr-based spintronics.

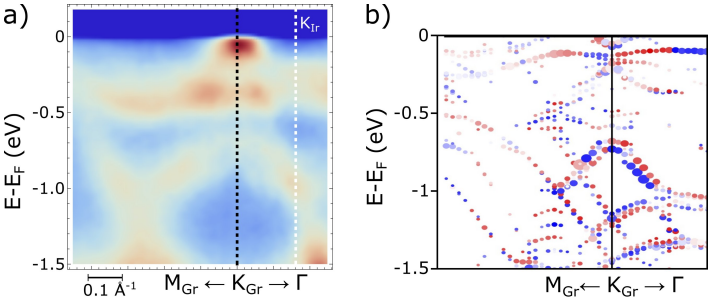

Figure 1: a) ARPES measurement of Gr/Pd/Ir(111). b) DFT simulations of the band structure of Gr/Pd/Ir(111).

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V5S8 under high pressure: a two-channel Kondo system?

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The layered system V5S8 displays a peculiar ground state characterized by the coexistence of metallicity with long-range antiferromagnetic order below T_N=32 K[1], where the magnetic V^{3+} ions are intercalated between adjacent metallic VS_2 layers[2]. The stability conditions of this ground state remains to be established; one scenario is that the antiferromagnetic order is driven by the conduction-electron-mediated Ruderman-Kittel-Kasuya-Yoshida (RKKY) interaction.

In order to verify this scenario and to investigate the interplay between conduction electrons and localized magnetic moments, we have studied the magneto-transport properties of single crystals as a function of pressure as control parameter. We find a rapid suppression of antiferromagnetism by pressure, concomitant with a dramatic increase of negative magnetoresistance. These results are explained by the increasing contribution of the Kondo effect competing with the RKKY interaction due to the enhancement of exchange interaction, J, with pressure, which opens the possibility of 2-channel Kondo behavior in layered dichalcogenides.

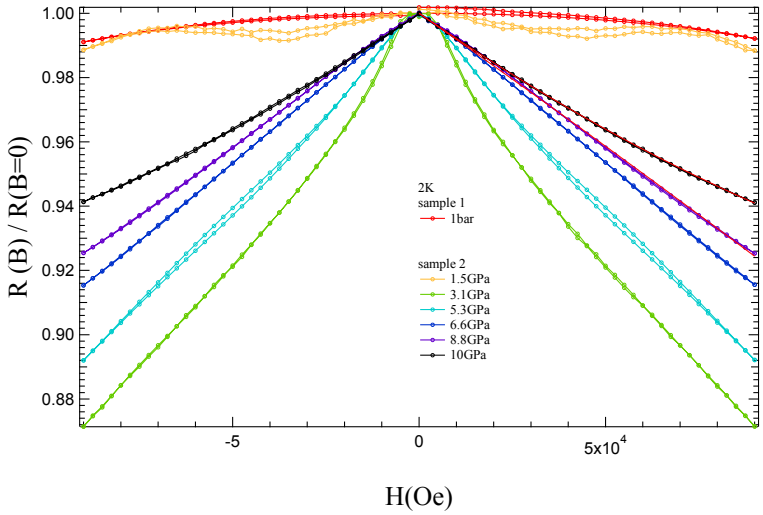

Figure 1 Magneto-resistance of V_5S_8 under high pressure at 2K

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