

Quantum Matter Bordeaux (QMBx)

QMBx Lecture Series: Colloquium, 22nd of October 2020

A. Pacault amphitheater (Centre de Recherche Paul Pascal)

The "Quantum Matter Bordeaux" (QMBx) programme supported by the department of "Material and Light Sciences" of the University of Bordeaux has for mission to federate research activities around subjects related to superconductivity, magnetism, functional materials, molecule-based magnets, heterostructures, nano-opto-mechanics, quantum chemistry, cold atoms, light-matter couplings, quantum technologies...

In the frame of the QMBx programme, we are organizing an international colloquium on the afternoon of Thursday **October 22nd**, in the Pacault amphitheater of the **Centre de Recherche Paul Pascal** (40 seats are "Covid" available). This colloquium can be chosen as part of the formation for PhD students of the doctoral schools of the Chemical Sciences (ED-SC), and Physics and Engineering (ED-SPI). Please register by email to quantum-matter.bureau@diff.u-bordeaux.fr before **October 19th** (a Zoom connection will also be provided).

The scientific program is given below (each 35 min talk will be followed by 15 min of questions and a 10 min break) and please don't hesitate to contact the visitors or their hosts if you want to meet them.



 **at 2 pm: "Integration of quantum chemistry methods in analysis of molecular magnetic properties"**

Dr. Elizaveta Suturina (University of Bath, UK; es2037@bath.ac.uk)

Visit from the 11-25th of October 2020

Contact person: Rodolphe Clérac (CRPP): clerac@crpp-bordeaux.cnrs.fr



 **at 3 pm: "Metal-insulator transitions in the spin-orbit Mott insulator Sr₂IrO₄ investigated by angle-resolved photoemission"**

Prof. Véronique Brouet (Laboratoire de Physique des Solides, Orsay, France; veronique.brouet@u-psud.fr)

Visit from the 19-23rd of October 2020

Contact person: Sébastien Burdin (LOMA): sebastien.burdin@u-bordeaux.fr



 **at 4 pm: "Superconducting nickelates"**

Dr. Andrés Cano (Néel Institute CNRS & UGA, Grenoble, France; andres.cano@neel.cnrs.fr)

Visit from the 21-23rd of October 2020

Contact person: Sophie Tencé (ICMCB): sophie.tence@icmcb.cnrs.fr



 **at 5 pm: "Collective excitations in twisted bilayer graphene"**

Prof. Marco Polini (Università di Pisa & Graphene Labs Genova, Italy and University of Manchester, UK; marco.polini@icloud.com)

Visit from the 19-23rd of October 2020

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at 2 pm: "Integration of quantum chemistry methods in analysis of molecular magnetic properties": Quantum chemistry has become a useful tool for understanding and predicting properties of molecules and materials from the first principles of quantum mechanics. Prediction of magnetic properties is one of the most challenging tasks for quantum chemistry, and yet it plays important role in the developing field of molecular magnetism. In this talk, I will show how quantum chemistry unveils the subtle differences in electronic structure of paramagnetic metal complexes that can create magnetic memory in a molecule. I will also present our latest studies of interactions between paramagnetic metal centres in complexes^[1] and extended networks,^[2] and how modulation of those interactions can turn a metal-organic framework into a room-temperature molecular magnet.^[2]

[1] X. Ma, E. A. Suturina, S. De, P. Négrier, M. Rouzières, R. Clérac, P. Dechambenoit, *Angew. Chem. Int. Ed.* (2018) 57, 7841; X. Ma, E. A. Suturina, M. Rouzières, M. Platinov, F. Wilhelm, A. Rogalev, R. Clérac, P. Dechambenoit, *J. Am. Chem. Soc.* (2019), 141, 7721

[2] P. Perlepe *et al.*, *Science* (2020), *in press*.

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at 3 pm: "Metal-insulator transitions in the spin-orbit Mott insulator Sr₂IrO₄ investigated by angle-resolved photoemission": Mott insulators are systems where electronic correlations are so strong that they localize electrons at integer fillings. The family of cuprates, famous for their high temperature superconductivity, are Mott insulators when they are not doped. It is widely believed that it is essential to understand how doping this Mott insulator proceeds to understand high temperature superconductivity. More recently, spin-orbit Mott insulator states have been discovered in 5d transition metals, where both spin-orbit and correlations are strong, setting a new background to study this physic. I will review the case of Sr₂IrO₄, with a special focus on metallic states obtained by doping. The insulator to metal transitions can be of different types and the changes in the electronic band structure are followed thanks to angle-resolved photoemission measurements.

Prof. Véronique Brouet (Laboratoire de Physique des Solides, Orsay, France; veronique.brouet@u-psud.fr)

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at 4 pm: "Superconducting nickelates": The recent discovery of superconductivity in the so-called infinite-layer nickelates has attracted an enormous research interest due to the analogies and differences with the high- T_C cuprates.^[1,2] I will provide an outlook of the superconducting properties of these d^9 systems from their electronic structure and discuss their degree of correlation.^[3,4] In addition, I will show that the fragile thermodynamic stability of these nickelates leads to specific interfacial effects^[5] and briefly discuss candidate materials for providing an ideal d^9 configuration.^[6]

[1] D. Li *et al.*, *Nature* (2019) 572, 624.

[2] M. R. Norman, *Physics* (2020) 13, 85, and the references therein.

[3] F. Bernardini, V. Olevano, A. Cano, *Phys. Rev. Research* (2020) 2, 013219.

[4] V. Olevano, F. Bernardini, X. Blase, A. Cano, *Phys. Rev. B* (2020) 101, 161102(R).

[5] F. Bernardini, A. Cano, *J. Phys. Mater.* (2020) 3, 03LT01.

[6] F. Bernardini, V. Olevano, X. Blase, A. Cano, *J. Phys. Mater.* (2020) 3, 035003.

Dr. Andrés Cano (Néel Institute CNRS & UGA, France;
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at 5 pm: "Collective excitations in twisted bilayer graphene"

Several experimental probes have been used to explore the physics of twisted bilayer graphene (TBG), including electronic transport, quantum capacitance, and scanning tunneling spectroscopy. However, probes that access the response to finite in-plane momentum q and frequency ω are expected to be rich sources of information in systems where electron-electron interactions play a dominant role. One of these probes is scattering near-field optical microscopy (SNOM), which enables the measurement of the dispersion relation of collective electronic excitations, such as Dirac plasmons in graphene. In this talk, I will discuss how SNOM can unveil the collective modes of electrons roaming in TBG^[1] and present a theoretical approach^[2] to calculate their spectra. I will try to argue that near-field optical probes offer new insights, complementary to those offered by other techniques, on the carrier dynamics in this correlated electron system.

[1] N. C.H. Hesp, I. Torre, D. Rodan-Legrain, P. Novelli, Y. Cao, S. Carr, S. Fang, P. Stepanov, D. Barcons-Ruiz, H. Herzig-Sheinfux, K. Watanabe, T. Taniguchi, D. K. Efetov, E. Kaxiras, P. Jarillo-Herrero, M. Polini, and F. H. L. Koppens, *arXiv:1910.07893*.

[2] P. Novelli, I. Torre, F. H. L. Koppens, F. Taddei, and M. Polini, *Phys. Rev. B* (2020) 102, 125403.

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Prof. Marco Polini (Dipartimento di Fisica del l'Università di Pisa & Istituto Italiano di Tecnologia, Graphene Labs, Genova, Italy and School of Physics & Astronomy, University of Manchester, UK; marco.polini@icloud.com)

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