

# Mini-rencontre du GDR Meeticc

Vendredi 04 Juin 2021  
De 13h30 à 15h30

Le lien générique pour vous inscrire à la réunion du 4 Juin est le suivant :

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## Programme

\*Animateur : Prénom **NOM**, laboratoire

	<i>Exposé (30 min + 10 min)</i>
13:30 – 14:10	<b>Rb<sub>2</sub>Ti<sub>2</sub>O<sub>5</sub>: a colossal permittivity solid electrolyte</b> Brigitte LERIDON CNRS/ESPCI Paris
	<i>Exposés (15 min + 5 min)</i>
14 :10 – 14 :30	<b>Lattice softening at the electric field and pressure-induced Mott insulator to metal transitions</b> Danylo BABICH Institut des Matériaux Jean Rouxel, Université de Nantes
	<i>Pause / discussion libre</i>
14:45 – 15 :05	<b>Quadrupolar effect in terbium pyrochlores</b> Yann ALEXANIAN Institut Néel, CNRS-Université Grenoble Alpes, Grenoble
15 :05 – 15:25	<b>Nematic insulator in twisted bilayer graphene</b> Eric BRILLAUX Laboratoire de physique, ENS Lyon
15:25 – 15:40	<b>Caractérisation de la position des oxygènes en couche mince via la diffraction résonnante</b> Antonio PENA-CORREDOR IPCMS

<b>First NAME : Brigitte</b>	<b>last NAME : LERIDON</b>
<b>Affiliation : CNRS/ESPCI Paris</b>	
Presentation type : <i>Long (30 min)</i>	Talk given in : <i>English</i> (please prepare the of the presentation in english)
I authorize the GDR to record a video of my presentation : <i>Yes</i>	

## **Rb<sub>2</sub>Ti<sub>2</sub>O<sub>5</sub>: a colossal permittivity solid electrolyte**

M<sub>2</sub>Ti<sub>2</sub>O<sub>5</sub> (where M= Rb, K,...) is a member of the Andersson-Wadsley titanate family. Firstly synthesized in the sixties, these compounds were initially noticed for their unusual titanium fivefold coordinence [1]. More recently, they have gained renewed interest for their remarkable electrical properties. In particular when Rb<sub>2</sub>Ti<sub>2</sub>O<sub>5</sub> is placed between two metallic electrodes under ambient atmosphere, it displays an equivalent permittivity at low frequency of about 10<sup>8</sup>, which opens the possibility to design supercapacitors with very high capacitance [2,3]. Similar results were also obtained on K<sub>2</sub>Ti<sub>2</sub>O<sub>5</sub> with a typical permittivity of 10<sup>7</sup> at room temperature [4]. Electrically, the system behaves like a non-transverse memristor [5].

Rb<sub>2</sub>Ti<sub>2</sub>O<sub>5</sub> was actually identified as a superionic conductor with an ionic conductivity of about 10<sup>-3</sup> S.cm<sup>-2</sup> [2,3]. However superionic conductors with equivalently high ionic conductivity are not known to exhibit colossal permittivity, which led us to investigate the microscopical mechanisms at play in the material.

In this presentation, I will discuss the physical characteristics of this type of solid electrolyte and its peculiarities.

In particular, charge distribution measurements have enabled us to show that the material, when placed under voltage, experiences a transition from an electronic insulator to an electronically conducting state near the cathode, which can be viewed as a virtual cathode entering the sample [6].

Remarkably, the mobile ions responsible for the remarkable properties of RTO are shown to come from water vapor incorporated into the sample [7]. I will discuss the possible microscopical models for the incorporation of water, the ionic transport and the accumulation of charges. I will also discuss the interest of these materials for « green » and cheap energy storage.

### **Références :**

- [1] S. Andersson and A. D. Wadsley, *Nature* 187, 499 (1960); S. Andersson and A. D. Wadsley, *Acta Chem. Scand.* 15, 663 (1961).
- [2] R.Federicci, S. Holé, A. F. Popa, L. Brohan, B. Baptiste, S.Mercone and B. Leridon, *Physical Review Materials* 1, 032001(R) (2017)
- [3] R. Federicci, B. Baptiste, F. Finocchi, A.F. Popa, L. Brohan, P. Giura, G. Rouse, A. Descamps-Mandine, T. Douillard, A.Shukla and B. Leridon, *Acta Cryst.* B73, 1142 (2017)
- [4] R. Rani, S. De Sousa Coutinho, S. Holé and B. Leridon, *Materials Letters*, 258, 126784 (2020)
- [5] R. Federicci, S. Hole, V. Démercy, and B. Leridon, *Journal of Applied Physics*, 124 ,152104 (2018)
- [6] S. de Sousa Coutinho, R. Federicci, S. Holé and B. Leridon, *Solid State Ionics*, Volume 333, 72-75 (2019)
- [7] S. de Sousa Coutinho, D. Bérardan, G. Lang, R. Federicci, P. Giura, K. Beneut, N. Dragoe, S. Holé and B. Leridon, *Solid State Ionics* 364, 115630 (2021)

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Presentation type : <i>Short (15 min)</i>	Talk given in : <i>English</i> (please prepare the of the presentation in english)
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## **Lattice softening at the electric field and pressure-induced Mott insulator to metal transitions**

*D. Babich, L. Cario, B. Corraze, C. Adda, J. Tranchant, M.-P. Besland, J.-Y. Mévellec,  
P. Bertoncini, B. Humbert and E. Janod*

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Mott insulators are a class of strongly correlated materials with emergent properties important for modern electronics applications<sup>[1]</sup>. The key property for potential application is the Mott insulator to metal transition (IMT). This IMT appears at equilibrium by submitting Mott insulators to various external perturbations such as pressure or electronic doping. However, the breakthrough concerning applications comes from recent discoveries showing the possibility of inducing out-of-equilibrium Mott IMTs thanks to light or electrical pulses which generate highly excited electronic states. On the theoretical side, the full description of Mott IMTs is a long-standing problem. At equilibrium, the evolution of most of the electronic properties at the Mott IMT can be well captured by the Hubbard Hamiltonian, a purely electronic model ignoring the response of the lattice.[2,3]. Conversely the description of out-of-equilibrium Mott IMTs is still a major theoretical challenge because of complex many-body effects and constitutes a very active field of research at present [4].

The paradigmatic example of Mott insulator is the  $(V_{1-x}Cr_x)_2O_3$  system. In this compound, an IMT can be induced at equilibrium by physical or chemical pressure and out-of-equilibrium by strong electronic excitation [5,6]. We have recently demonstrated that a local lattice contraction accompanies the out-of-equilibrium Mott IMT caused by an electric field [7], which is reminiscent of  $\approx 1\%$  volume drop observed at the Mott IMT observed at equilibrium under pressure [6].

During the talk, we will present Raman studies on  $(V_{1-x}Cr_x)_2O_3$ , showing that, despite the lattice contraction, the Mott IMT is associated to a softening of elastic constants, both at equilibrium (chemical and physical pressure-induced IMT) and out-of-equilibrium (E-field-induced IMT). These results show that the minimal model to fully describe the Mott IMT in solids is a Hubbard model on a compressible lattice. Most importantly, this work also illustrates how the degree of the electronic delocalization can control the lattice stiffness in strongly correlated systems, [7,8] both at and out-of thermodynamic equilibrium.

### **Références :**

- [1] E. Janod *et al.*, *Adv. Funct. Mater.* **2015**, 25, 6287.
- [2] V. I. Anisimov, J. Zaanen, O. K. Andersen, *Phys. Rev. B* **1991**, 44, 943.
- [3] J. Hubbard, Proceedings of the Royal Society of London A: Mathematical, Physical and Engineering Sciences **1964**, 281, 401
- [4] Aoki *et al*, *Reviews of Modern Physics*, 2014, Vol. 86, Iss. 2
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- [7] S. Populoh, P. Wzietek, R. Gohier, P. Metcalf, *Phys. Rev. B* **2011**, 84, 075158.
- [8] I. Leonov, V. I. Anisimov, D. Vollhardt, *Phys. Rev. B* **2015**, 91, 195115.

<b>First NAME : Eric</b>	<b>last NAME : BRILLAUX</b>
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Presentation type : <i>Short (15 min)</i>	Talk given in : <i>English</i> (please prepare the presentation in English)
I authorize the GDR to record a video of my presentation : <i>YES</i>	

### **Nematic insulator in twisted bilayer graphene**

Twisted bilayer graphene has spurred a tremendous research activity since the discovery in 2018 of correlated phases (notably insulating and superconducting) at special ‘magic’ angles. In twisted bilayer graphene, two layers of graphene overlap with a small relative twist in such a way that the lattice mismatch generates a large moiré pattern whose unit cell can comprise tens of thousands of atoms. The interplay between interlayer tunneling and the moiré geometry leads to an unusual ‘magic’ angle physics: at a discrete set of so-called ‘magic’ twist angles, the Fermi velocity of the Dirac cones vanishes, and the energy bands flatten out dramatically, which enable many-body effects to dominate the electronic properties. Among the plethora of correlated phases observed at the magic angle, a strong insulating state develops at charge neutrality, which also breaks the three-fold rotational symmetry of the moiré pattern, leading to a so-called ‘nematic’ insulator. In this work, we first build a continuum model for the low-energy physics at charge neutrality, and determine the correction to the Fermi velocity perturbatively in the tunneling strength. We then classify all contact interactions allowed by symmetry, and develop a renormalization group approach to study the competition between the relevant instabilities. We show that the proximity to the magic angle favors indeed the formation of a gap and the breaking of the three-fold rotational symmetry.

#### **Références :**

Brillaux, E., D. Carpentier, A. A. Fedorenko, and L. Savary (Aug. 2020). “Nematic insulator at charge neutrality in twisted bilayer graphene”. arXiv:2008.05041

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Presentation type : <i>Short (15 min)</i>	Talk given in : <i>English</i> (please prepare the presentation in English)
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## **Caractérisation de la position des oxygènes en couche mince via la diffraction résonnante**

Les oxydes en couche mince sont un sujet de plus en plus attrayant en raison de leurs potentielles applications en spintronique et/ou en orbitronique. Les propriétés de ces systèmes sont fortement dépendantes de la structure cristalline qui est liée à l'ordre orbitaire (OO) du composé [1] [2]. Par conséquent, la résolution structurale des couches minces est nécessaire à la détermination des OO.

Contrairement aux matériaux massifs, où les techniques « classiques » de diffraction permettent de localiser les différents atomes qui composent le cristal [3], les couches minces ont beaucoup moins de matière à sonder, rendant ces techniques difficilement exploitables. Une alternative à ce problème est l'utilisation de la diffraction résonnante des rayons X (REXS) aux seuils d'absorption. Cette technique, traditionnellement effectuée sur la partie XANES (*X-ray Absorption Near Edge Structure*) du spectre, s'est avérée efficace pour sonder les cations métalliques dans des couches minces d'oxyde [4]. L'utilisation du REXS de manière analogue au seuil de l'oxygène pour caractériser les ligands n'est cependant pas envisageable du fait de sa longueur d'onde trop importante ( $\lambda \approx 20\text{\AA}$ ).

Pour déterminer les positions de l'oxygène, nous proposons une méthode reposant sur l'étude des spectres REXS acquis aux seuils des cations dans le domaine comprenant les parties XANES et aussi EXAFS (*Extended X-ray Absorption Fine Structure*). Cette dernière partie des spectres est en effet sensible à l'environnement électronique de l'atome sondé [5] et, par conséquent, sera influencée par les positions des oxygènes voisins. En utilisant le logiciel FDMNES [6], nous avons prouvé par une approche numérique la possibilité d'ajuster les spectres EXAFS et de déterminer la position des oxygènes sur l'oxyde  $\text{FeV}_2\text{O}_4$  de structure spinelle. Cette approche, valable à la fois pour les matériaux massifs et en couche mince, a pour but d'être généralisée à tous les systèmes. Le développement de cette technique permettra de caractériser la cristallographie dans un film cristallin, ce qui est nécessaire à la conception des futurs dispositifs pour l'orbitronique.

### **Références :**

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