CEA - Saclay 91191 Gif-sur-yvette Cedex
Service de Physique de l'Etat Condensé
SÉMINAIRE THEMATIQUE
Jeudi 16 octobre 2014 à 11h15

Orme des Merisiers SPEC, Salle Itzykson, Bât.774

Topological phases in bismuth compounds

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Topological insulators are a newly discovered class of materials which are bulk insulators with metallic surface states. The existence of gapless surface states is a direct consequence of the non-trivial topology of the bulk band structure of these materials. As a result theses states are robust against local disorder and currents propagate without back-scattering from non-magnetic defect. These exceptional electronic properties open the possibility to realize new phenomena in condensed matter physics ranging from fundamental physics (Majorana fermions) to technological applications (quantum computing, spintronics).

In Z_2 topological insulators, the topological phase originates from time reversal symmetry and strong spin-orbit interaction. As a consequence, bismuth, which is the stable element with the highest spin-orbit coupling strength, is a key ingredient of many topologically non-trivial compounds. Two well-known examples of such compounds are Bi_2Se_3 and Bi_2Te_3 which are strong topological insulators with Dirac surface states.

Here I will present a density functional theory (DFT) study of other bismuth compounds with interesting topological phases. I will first discuss the case of BiTeI, a layered semiconductor with giant Rashba splitting [1] which is expected to undergo a topological phase transition under pressure. It was predicted that pressure lead to gap closure with further reopening resulting in a strong Z_2 topological insulator type band structure [2]. Using GW approximation calculations we show that the predicted topological phase transition is hindered by the structural phase transition taking place at a lower pressure [3]. I will then discuss this discovery of a new topological phase in the quasi one-dimensional compound Bi_4I_4. While DFT predicts a weak topological phase, the correct estimation of band ordering using the GW approximation reveals this material is a strong topological insulator characterized by Z_2 invariants (1,110). The existence of this strongtopological phase is con_rmed experimentally using ARPES.

Reference:
[1] A. Crepaldi et al., Phys. Rev. Lett. 109, 096803 (2012).
[2] M.S. Bahramy, B.-J. Yang, R. Arita, and N. Nagaosa, Nature Commun. 3, 679 (2012).
[3] M. K. Tran et al., Phys. Rev. Lett. 112, 047402 (2014).

A coffee break will be served at 11h00. The seminar will be given in English.