Materials Science and Technology Division
Materials Theory Group

"Possible pressure-induced topological insulating phase in BiTeI"

Ryotaro Arita
The University of Tokyo, Japan

Wednesday, March 7, 2012
11:00 a.m.
4515/HTML, Room 265

Abstract

Recently, it has been experimentally discovered that bulk BiTeI has a giant Rashba-type spin splitting. [1] In this talk, we first discuss how the huge splitting appears in this compound. We propose that there are three key conditions: (i) strong spin-orbit interaction in a non-centrosymmetric system, (ii) a narrow band gap, and (iii) presence of top valence and bottom conduction band of symmetrically the same character. [2] We then show through first-principles density functional calculation that BiTeI turns into a topological insulator by applying pressure, and discuss what kind of unique features it should have. [3]

[1] K. Ishizaka et al., Nature Materials 10 521 (2011)
[2] M.S. Bahramy, R. Arita and N. Nagaosa, Phys. Rev. B.84 041202(R) (2011)
[3] M.S. Bahramy, B.-J. Yang, R. Arita and N. Nagaosa, Nature Communications 3, 679 (2012)

Host: Di Xiao (576-0301, xiaod@ornl.gov)