Emergent phenomena in giant bulk Rashba semiconductors

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In this talk, I will overview our recent theoretical and experimental studies on giant bulk Rashba semiconductors. In these materials, the bulk electronic states exhibit extremely large Rashba spin splitting, due to the strong spin-orbit interaction of electrons and the intrinsic bulk polarity of the systems. Backed by our first-principles calculations, we have observed this phenomenon in a group of Bismuth Tellurohalides [1-3]. After briefly describing the electronic structure of these systems, I will discuss the origin of giant bulk RSS based on the group theory and *k.p* formalism [3]. Three conditions will be shown to be necessary for realization of giant bulk Rashba splitting. These conditions are (i) large atomic spin-orbit interaction in an inversion-asymmetric environment, (ii) a narrow energy gap between the conduction and valence bands, and (iii) the similarity between the symmetry characters of top valence bands with that of bottom conduction bands. Of particular importance, the third criterion is fulfilled by an unconventional ordering of bands in all Bismuth Tellurohalides, resulting from the negative crystal field splitting of the top valence bands. I will also show that as a result of giant bulk Rashba spin splitting, these materials exhibit a divergent orbital dia/para-magnetism, controllable by electron doping [4]. We observe a large temperature-dependent diamagnetic susceptibility when the Fermi level is slightly above the crossing point of Rashba-split conduction bands. On the other hand, the susceptibility turns out to be paramagnetic when the Fermi level is below the crossing point. Two mechanisms are proposed to be responsible for the enhanced paramagnetic susceptibility. The bulk Rashba splitting will also be shown to lead to some unique features in the optical conductivity and magneto-optical responses, resulting from the inter and intra-band transitions [5,6]. I will finally discuss the possibility to induce an unconventional topological phase transition in these systems [7]. Our strategy for this is to modify the chemical bonds, and thus the crystal field splitting by applying a hydrostatic pressure. It will be demonstrated that at a critical pressure the band gap fully closes at certain *k*-points and at higher pressures, the system becomes a strong topological insulator. Interestingly, the topological surface states have completely different dispersions at top and bottom sides; at one side Dirac point is buried within the bulk valence continuum while at the other side it is inside the bulk band gap. The topological phase transition in these systems will be shown not to be describable by the available theories as they expect the topological phase transition in non-centrosymmetric systems to be mediated through a range of pressures rather than at a single critical pressure and, furthermore, within this range the system should remain gapless. To address this issue, we have constructed a general theory, successfully describing the topological quantum phase transitions in 3D systems with broken inversion symmetry. According to our theory, in such systems a direct phase transition from a normal insulator to a topological insulator can occur if the accidental band crossing occurs along directions with high crystalline symmetry [8].

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