Antiferromagnetic Topological Insulator: Theory and Material Design

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By using staggered electric potential, antiferromagnetic exchange field and spin-orbit coupling, we can control the spin, valley and sublattice degrees of freedom of electrons on honeycomb lattice, and achieve a novel topological insulator with simultaneous finite charge and spin Chern numbers. With first-principles calculation we demonstrate that the scheme can be realized in a sandwich of $[LaCrO_3]_n/La_2Au_2O_6/[LaCrO_3]_n$ along [111] direction of the perovskite structure. The d8 electrons of Au^{+3} hop on a buckled honeycomb lattice and exhibit Dirac behaviors, which feel the antiferromagnetic exchange field from bulk $LaCrO_3$, a Mott insulator with G-type antiferromagnetic order. The staggered electric potential on d8 electrons is provided by an electric field along [111] direction taking advantage of the buckling structure of honeycomb lattice. Due to the orbit hybridization, spin-orbit coupling is enhanced to 30meV, which hopefully makes the topological state stable even up to room temperature. In a finite system, there appears a quantized edge current with full spin polarization, while the total magnetization is compensated to zero. In this topological half-metallic antiferromagnet (HMAFM), the spin polarization of the dissipationless edge current can be inverted by gate voltage, which is a tremendous advantage in spintronic applications.

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[1] Q.-F. Liang, L.-H. Wu and X. Hu: NJP 15, 063031 (2013)
[2] X. Hu: Adv. Mater. 24, 294 (2012).