Novel Topological State in Perovskite Materials

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Abstract

A topological state called antiferromagnetic topological insulator characterized by simultaneous nonzero charge and spin Chern numbers is possible for electrons on honeycomb lattice based on band engineering by staggered electric potential and antiferromagnetic exchange field in presence of intrinsic spin-orbit coupling. With first principles calculation we confirm that one can achieve this new state by inserting a [111] mono-atomic layer of gold (Au) into a Mott insulator $LaCrO_3$ of perovskite structure and applying an electric field along [111] direction. This material is ideal for spintronics applications, since a finite sample provides a spin-polarized quantized edge current, robust to both nonmagnetic and magnetic defects, with the spin polarization tunable by electric field [1]. The total magnetization is compensated to zero, and thus the system can be considered as a half-metallic antiferromagnet [2-4].

Topology becomes the central concept in condensed matter physics and material science. The breakthrough took place when Kane and Mele clarified that electrons on graphene, a two-dimensional honeycomb lattice of carbon atoms, open a gap by spin-orbit coupling (SOC) and achieve a topologically nontrivial state called quantum spin Hall effect (QSHE) [5]. This discovery triggers a huge amount of activities in exploring topological states and materials.

As the common home base for both Kane-Mele model [5] and the spinless Haldane model [6], honeycomb lattice serves a unique role in understanding the topological property of electron systems. It may be illustrative to summarize its electronic structure paying attention to the Berry curvature configuration. There are two sites in the unit cell of honeycomb structure. With nearest neighbor hopping, electronic valance and conduction bands touch linearly and thus form Dirac cones at two inequivalent k points, K and K', locating at the corners of Brillouin zone. It is important to observe that Bloch wave functions exhibit opposite chiral features around K and K', characterized by opposite Berry curvatures (see Fig. 1), which establishes the special position of honeycomb lattice in exploring topological state. By using spin-orbit coupling, the antiferromagnetic exchange field and the staggered electric potential, we can reverse the Berry curvature at for example K’ point in spin-down channel, resulting in a topological state characterized by simultaneous nonzero charge and spin Chern numbers [1,7]. The band engineering is based on a full control on the degrees of freedom of spin, valley and sublattice. Since the staggered magnetic field can be realized by antiferromagnetic (AFM) insulators, compact and stable devices based on the topological state in Fig. 2(e) are possible as compared with the photo-assisted scheme [7].

As material realization of our idea, we focus on d-electron systems in perovskite structure. First, we choose a perovskite insulator $LaCrO_3$ with G-type AFM order on the magnetic Cr atoms. Along [111] direction Cr atoms form a stacking of buckled honeycomb lattices, which can be grown by cutting-edge molecular beam epitaxial (MBE) with atomic precision. During the growing process, a single buckled honeycomb layer of Cr atoms is replaced by that of nonmagnetic Au atoms, where the element Au is chosen conjugate to Cr in order to form a d^8 configuration. For Au-d electrons on the single buckled honeycomb lattice, intrinsic SOC becomes sizable, a uniform electric field along [111] direction induces a staggered electric potential for the two sublattices, and the G-type AFM order on Cr atoms on the two sides provides an AFM exchange field. The material design makes the magnetic field of pure exchange character. We have checked successfully our idea by performing first principles calculations for several materials. In transition metal perovskites we found intrinsic SOC of several tens of meV, which is larger than that in silicene in magnitude by one or two orders, and makes the new topological state available even above room temperature.

Acknowledgements

This work was supported by the WPI Initiative on Materials Nanoarchitectonics, MEXT, Japan, and partially by a Grants in Aid for Scientific Research (No. 22540377), JSPS, and Innovative Area “Topological Quantum Phenomena” (No.25103723), MEXT of Japan.

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Figures

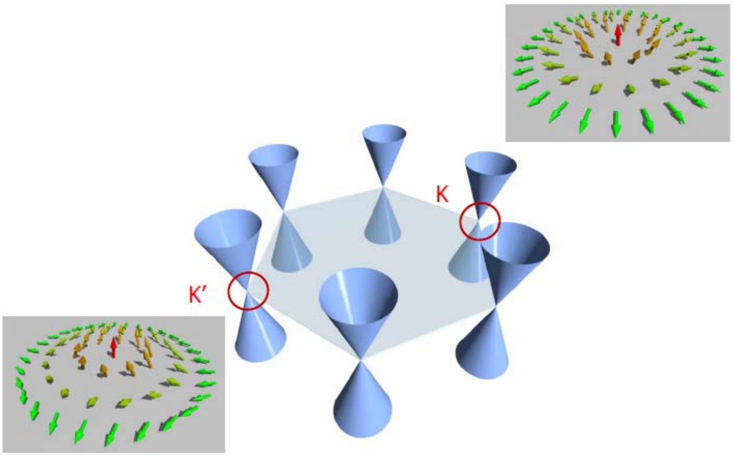

Fig. 1: Dirac cones and merons of structure for electrons on honeycomb lattice.

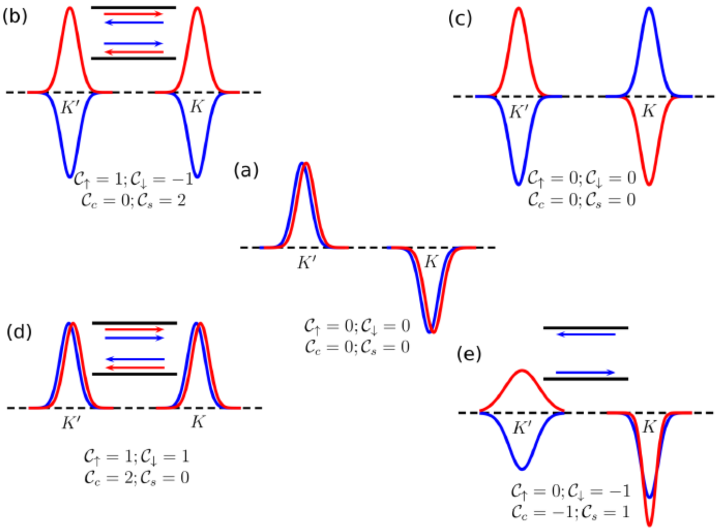

Fig. 2: Possible configurations of Berry curvatures for electrons on honeycomb lattice [1]: (a) pristine honeycomb lattice under staggered electric potential; (b) QSHE; (c) SDW; (d) QAHE; (e) novel topological insulator state addressed in the present talk [1,7].