Sizable Band Gap In Organometallic Topological Insulator

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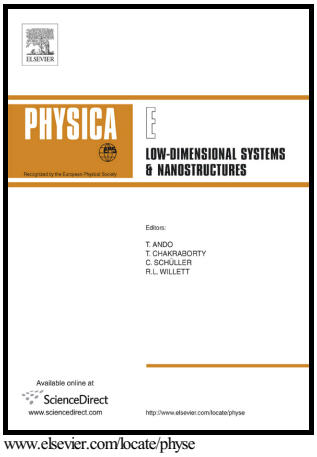

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Sizable Band Gap In Organometallic Topological Insulator

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Abstract

Based on first principle calculation when Ceperley-Alder and Perdew-Burke-Ernzerh type exchange-correlation energy functional were adopted to LSDA and GGA calculation, Electronic properties of organometallic honeycomb lattice as a two-dimensional Topological insulator was calculated. In the presence of spin-orbit interaction bulk band gap of organometallic lattice with heavy metals such as Au , Hg , Pt and Tl atoms were investigated. Our results show that the organometallic Topological insulator which made of Mercury atom shows the wide bulk band gap about ~ 120 meV. Moreover, by fitting the conduction and valence bands to the band-structure which produced by Density Functional Theory, spin-orbit interaction parameters were extracted. Based on calculated parameters, gapless edge states within bulk insulating gap are indeed found for finite width strip of two-dimensional organometallic Topological insulators.

Keywords: Spin-orbit interaction, Organometallic lattice, Topological insulator, Edge states, Density Functional Theory

1. Introduction

Topological insulators (TI) have ignite great attractions in the field of condensed matter physics and material science as it constitutes a newly discovered phase of matter. TIs are a class of materials exhibiting unique quantum transport features with potential applications in field of spintronics and quantum computing [1, 2, 3, 4, 5]. TIs have a bulk insulating band gap as do normal insulators but they have protected conducting edge states for two dimensions (2D) and surface states for three dimensions. The Z_2 topological insulator is characterized by an odd number of gapless modes per edge that are robust against weak non-magnetic perturbations preserving the time-reversal (TR) symmetry. The existence of such gapless edge states is generally guaranteed by a general theorem under the name of bulk/edge correspondence [6, 7]. According to TR symmetry, the currents carried by the edge states are dissipationless. The existence of the TI phase was first proposed by Kane and Mele in graphene, in which spin-orbit interaction (SOI) opens a band gap at the Dirac points[8] . The interesting physics and potential applications for spin manipulation would not be manifested in the pure graphene, because the SOI in pure graphene is quite small [9]. silicene, the silicon-based successor of graphene, with buckled honeycomb geometry, has been synthesized through epitaxial growth[10]. This novel two-dimensional material has recently attracted considerable attention both theoretically and experimentally , due to its exotic electronic structure and promising applications in future nanoelectronics as well as its compatibility with current silicon-based electronic technology [11, 12, 13]. The bulk insulating SOI gap of silicene is 1.5 meV [5]. An excellent topological insulator material should have a large enough band gap and be easily fabricated. Since bulk insulating gap of mentioned TIs are yet relatively small therefore, it is crucial to search for materials with strong SOI to realize the topological phase. Newly, in order to find TIs with larger SOI insulating gap, based on the first-principle calculations, formation of 2D TI on Si$(1 \times 1 \times 1)$ surface with relatively large bulk band gap $\sim$ 0.8 eV has been predicted [14].

Recently, several generations of topological insulators have been theoretically predicted and experimentally confirmed, all based on inorganic materials [15, 16, 17, 18, 19, 20, 21]. Lately, organometallic TI as a new type of TI has attracted increasing attention from both theoretically and experimentally. Based on first-principle calculation it has been pointed out that organometallic honeycomb lattices is another plausible material for Quantum Spin Hall (QSH) effect[22, 23, 24]. This new class of TI exhibits nontrivial topological edge states. Wang et al., in [23] showed that turning on the SOI give rise to opening a gap of 8.6 meV which opens in location of high symmetry K point when Pb atom used as metal. Also when the Pb atom replaced with Bi bulk insulating gap as large as 43 meV opened up. Motivated by the increasing interest in finding larger spin-orbit bulk gap, we attempt to search an organometallic honeycomb lattice with heavy metals which exhibits the larger bulk insulating gap than those which introduced so far.

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