Rashba effects in surface-Bi nanostructures

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Systems exhibiting the Rashba effect is of fundamental importance due to their characteristic spin textures. The Rashba effect is possible not only in two-dimensional surface structures, but also in one-dimensional surface nanostructures. As a possible candidate for technological applications, spin-filtering exploiting the Rashba effect is promising, which is caused by band structures with opposite spin directions at the Fermi energy for the positive and negative electron momenta with each other. Even though such a band structure is proposed using an application of the magnetic field [1], it has not been realized yet without an external magnetic field. As a constituent element of the one-dimensional nanostructure, Bi is expected to be promising because of large spin-orbit coupling coming from its large atomic number.

In this study, we investigated a new one-dimensional Rashba system, Bi-adsorbed In atomic chains, using first-principles calculations [2]. First-principles calculations were performed on the basis of density functional theory with the generalized gradient approximation by the OpenMX code [3]. One of the most stable structures in the system shows unconventional spin textures, which is the reversal of the spin polarization direction in Rashba bands. This band structure is caused by a gap-opening due to the avoided-crossing of two Rashba bands. We have confirmed using a group-theoretical analysis that four relevant Rashba bands are classified into two irreducible representations as in Fig. 1 (a). The avoided-crossing is caused by the hybridization of two Rashba bands belonging to the same irreducible representation. The schematic representation of this hybridization is shown in Fig. 1 (b). Together with the shift of the Fermi level within the gap, our results suggest a new spin-filtering mechanism through atomic chains. In addition, our mechanism has a great advantage; previous spin-filtering mechanisms require the external magnetic field [1], whereas ours does not need the magnetic field. This feature is suitable for spintronic applications.

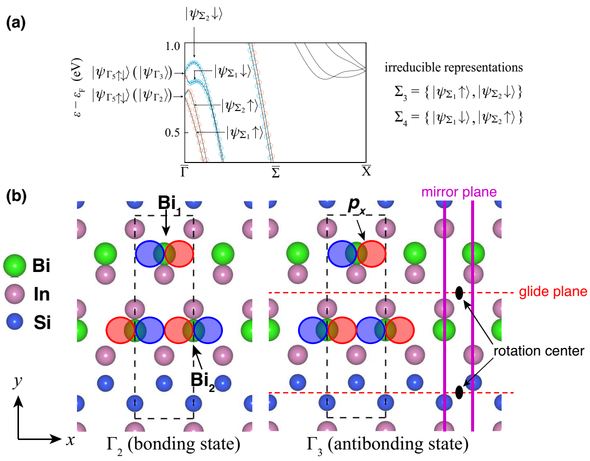

Figure 1: (a) Spin-polarization components parallel to the y axis as open circles with the band dispersion. The classification of the four Rashba bands into the irreducible representations are also shown. (b) Schematic illustrations of the hybridization together with the symmetry elements. The drawn orbitals represent p_x orbitals of Bi.

[1] C. H. L. Quay *et al.*, Nature Phys. **6**, 336 (2010).

[2] T. Tanaka and Y. Gohda, Phys. Rev. B **98**, 241409(R) (2018)

[3] T. Ozaki, Phys. Rev. B. **67**, 155108 (2003).