

# Applications of Double Group Theory in 2D Materials

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**Abstract**—Group theory is a fundamental mathematical framework valuable for analyzing the band structures in materials science. The hexagonal structures have unique electronic structures, especially in 2D materials in group-IV, where the system is observed as the topological insulator. Meanwhile, in the case of group-V, it is semiconductors. This paper analyzes group-IV and group-V band structures based on group theory and proposes a method to identify the irreducible representation (IR) in symmorphic systems. It is found that all materials in group-IV are topological insulators. The evaluation of  $Z_2$  invariant  $\nu$  in group-V found that the phosphorene and bismuthene cases are  $\nu = 0$  and  $\nu = 1$ , respectively, and belong to trivial and topological insulator materials for phosphorene and bismuthene, respectively.

**Index Terms**—Group Theory, 2D Materials, Group IV, Group V

## I. INTRODUCTION

Group theory is a branch of mathematics that uses powerful tools to describe the symmetry and structure of physical systems. In materials science, the symmetry and transformations of a crystal lattice or a molecular structure reflect the arrangement and organization of atoms or ions in an orderly spatial lattice. Those directly correlate with the materials' optical, electronic, and mechanical properties.

The crystal symmetry have depends on the rotation, translation, reflection and inversion that affect physical properties. The ground state of physical systems is measured by maximum symmetry due to attraction between its components, and thus, the ground state of the crystals should be invariant and respected to all operations of the group. The symmetry corresponds to conserved quantities and allows the classification of quantum mechanical state, including the representation theory and degeneracy or level splittings. The wave functions or operators determine the state; the set of the spectrum of an operator (eigenvalues) is discrete. Those means to measure the quantization phenomenon of the operators in discrete[1].

In the cases of 2D materials, group IV and group V have been attracting scientific interest due to their novelty[2], [3], [4], [5], [6]. Group IV forms hexagonal symmetries, which rotate  $2\pi/3$  at the  $z$ -axis. The hexagonal structure is found in Group V when the thickness is large[7], [8], [9], [10], [11]. The electronic structure characteristics of group IV have a Dirac cone; meanwhile, group V is semiconductors[2], [3], [12], [13], [14], [15], [16]. At the Dirac cone, the spin-orbit coupling splits the stick bands that affect to induces a

topological insulator. The materials containing heavy elements have large SOC and this materials is one of the candidates for topological materials[17], [18]. Furthermore, both groups are observed as topological insulators at different conditions.

To understand the electronic properties of 2D materials group IV and group-V, the band structure is analyzed based on double group theory. Identifying the irreducible representation (IR) of symmetric systems, including SOC, requires analyzing double group theory.

This research uses double group theory to analyze the IR band in order to study the 2D materials of group IV and group V. For consideration, the materials are graphene, silicene, germanene and stanene as group IV and phosphorene and bismuthene as group V, respectively. The proposed method to identify IR in non-SOC and SOC bands is discussed. The  $Z_2$  invariants are evaluated to observe the materials, including topological or trivial insulators.

## II. METHOD

The previous studies used the method to identify IR when non-SOC calculations are applied[15], [16], [19], [20], [21], [22]. It also reported that the technique for SOC calculations was used in the cases of symmorphic and non-symmorphic systems[23], [24]. Since the symmetry is hexagonal symmetry, the system belongs to symmorphic system.

First, introduced a method to identify the IR of the wavefunctions,  $\psi_{k,n}^\gamma$ .  $\gamma$  is two component of spinor Bloch wavefunctions. The band index in the ascending sequence of energy is  $n$ , and the wavevector in the first Brillouin zone is  $k$ . When the wavefunctions have the  $m$ -th degeneracy [3,4], we evaluate  $Q^\beta = \frac{1}{p} \sum_{a=n}^{n+m-1} \sum_i \chi^\beta(\hat{R}_i)^* \langle \psi_{\mathbf{k}}^a | \hat{R}_i | \psi_{\mathbf{k}}^a \rangle$ , where  $p$  is the order of the group and  $\chi^\beta(\hat{R}_i)$  is the character of the IR  $\beta$ .  $i$  runs over the symmetry operations  $R_i$ . The wavefunctions belong (do not belong) to the  $\beta$ -th IR when  $Q^\beta = 1$  ( $Q^\beta = 0$ ). The detailed explanation of the group theory in the non-SOC and SOC systems was observed in the previous papers[20], [23], [24].

The above methods are implemented to identify IR in the First-principles calculation PHASE/0 code[25]. First, the self-consistent calculation of the electronic structure of the crystal is calculated based on density functional theory using PHASE/0 code until the ground state occurs in both cases (non-SOC and SOC calculations). Then, calculate the band structure by considering the first Brillouin zone. Analyze the band structure results computed from PHASE/0 with Band\_Symm using group theory to identify the IRs to which the state belongs. TSPACE package is used to indices the IR

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meV) at  $\Gamma$ -point[24]. The calculate  $\nu=0$  consider to trivial insulator. On the contrary, the calculation of  $Z_2$  invariant in the case of bismuthene is  $\nu = 1$ . This is due to the large split band which is reversed the lowest unoccupied and highest occupied bands. Therefore, the  $Z_2$  invariant of 1 is because the strong SOC in heavy materials of group-V.

#### IV. CONCLUSION

To identify IR of the SOC wavefunctions using computers, a method based on double group theory succeeded in implementing it to analyze the band structures of two-dimensional systems group-IV and group-V. In the cases of group-IV, the two-dimensional IR are found in the Dirac cone of planar E" and buckled structures E. The SOC split those bands in planar graphene into  $E_{1/2}$  and  $E_{3/2}$  and  $E_{3/2}$  have lower energy than  $E_{1/2}$ . The SOC calculation of buckled structure group-IV split the Dirac cone into lower levels of  $e_{3/2}(1)$  and  $e_{3/2}(2)$  and  $E_{1/2}$ . The two levels,  $e_{3/2}(1)$  and  $e_{3/2}(2)$ , have the same energy due to time-reversal symmetry. On the other hand, the SOC split the  $E_g$  level of group-V into  $e_{3/2g}(1)$  and  $e_{3/2g}(2)$  and  $E_{1/2}$  which is the former has high energy than the latter. The large split energy in bismuthene case is shown to reverse the  $E_g$  level and  $e_{3/2g}(1)$  and  $e_{3/2g}(2)$  become unoccupied state. The evaluation of  $Z_2$  invariant  $\nu$  of group-IV is found that all materials are topological insulators. In the case of group-V, the trivial and topological insulators are detected in phosphorene and bismuthene cases, respectively. The topological insulator in group-V is observed that the large SOC affect the reverse band and the calculation of  $\nu=1$  as a topological insulator.

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