

Topological classification of crystalline insulators with space group symmetry

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We show that in crystalline insulators, space group symmetry alone gives rise to a topological classification based on the discretization of electric polarization. Using C_3 rotational symmetry as an example, we first prove that the polarization is discretized into three distinct classes, i.e., it can only take three inequivalent values. We then prove that these classes are topologically distinct. Therefore, a Z_3 topological classification exists, with polarization as a topological class index. A concrete tight-binding model is derived to demonstrate the Z_3 topological phase transition. Using first-principles calculations, we identify graphene on a BN substrate as a possible candidate to realize these Z_3 topological states. To complete our analysis, we extend the classification of band structures to all 17 two-dimensional space groups. This work will contribute to a complete theory of symmetry-conserved topological phases and also elucidate topological properties of graphenelike systems.

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I. INTRODUCTION

Since the celebrated discovery of the quantum Hall effect,¹ topological classification of electronic states has emerged as a powerful concept in condensed matter physics. Quantum Hall insulators are distinguished from ordinary insulators by a topological index, the Thouless-Kohmoto-Nightingale-Nijs (TKNN) number, which gives the quantized Hall conductance.^{2,3} For a long time, the TKNN number was thought to be the only topological index describing nondegenerate electronic ground states. Recently, it was realized that in crystalline insulators, new topological indices can be defined in the presence of discrete symmetries, which has led to the identification of a slew of new topological states. For example, quantum spin Hall insulators are characterized by a nontrivial Z_2 index,⁴ which is protected by time-reversal symmetry.^{5,6} Similarly, magnetic translation symmetry can also give rise to a Z_2 classification in antiferromagnetic insulators.⁷ Another interesting proposal is the so-called topological crystalline insulators, in which a Z_2 index can be defined and is protected by both time-reversal and certain point-group symmetries.^{8,9}

In this paper, we show that in crystalline insulators, space group symmetry *alone* can give rise to a new topological classification based on the discretization of electric polarization. Our idea is inspired by a beautiful result due to Zak¹⁰ and builds upon work done by Vanderbilt and King-Smith.¹¹ Zak showed that in one-dimensional (1D) systems with inversion symmetry, the Berry phase of the Bloch bands can be either 0 or π (Ref. 12) (when the origin is defined at the Wyckoff positions of the 1D crystal). This discretization of the Berry phase naturally leads to a Z_2 classification in one dimension. Later on, Vanderbilt and King-Smith¹³ showed that this property also carries over to higher dimensions, with the role of Zak's phase replaced by electric polarization.^{13,14} In this paper, we expand this idea by showing that under conservation of crystal symmetry, the discretized polarization can be used as a topological index. Recently, the role of crystal symmetry in the classification of topological matter has been discussed in several works.¹⁵⁻¹⁷

For the sake of definiteness, 2D crystals with C_3 rotational symmetry are used as an example in the following discussion. We first prove, from a general symmetry argument, that the polarization is discretized and can only take values belonging to three distinct classes. Therefore, a Z_3 topological classification exists. We then proceed by constructing a concrete tight-binding model to demonstrate the existence of various Z_3 topological states and the topological phase transition in the presence of C_3 symmetry. We prove that transition between distinct classes of polarization closes the band gap and is therefore topological in nature. Polarization is a useful topological index, as it is theoretically and experimentally easily accessible. Moreover, our result links the polarization values of all materials that are topologically equivalent under this classification. Using first-principles calculations, we identify graphene on a BN substrate¹⁸⁻²¹ as a possible candidate to realize the Z_3 topological states. The misconception that C_3 symmetry enforces zero polarization is also clarified. Finally, we extend our analysis to all space groups in two dimensions. Since a many-body formulation of the electric polarization already exists,^{22,23} the topological classification scheme discussed here can be readily applied to interacting systems.

II. GENERAL SYMMETRY ANALYSIS

The discretization of polarization under high crystal symmetry has been mentioned by Vanderbilt and King-Smith.¹¹ Here we discuss it using a concrete example of systems with C_3 rotational symmetry. Theoretically, it has been well established that the polarization in a crystal is formally defined only modulo a quantum uncertainty,^{13,14} i.e., the polarizations \vec{P} given in the following expression are all equivalent to each other:

$$\vec{P} \simeq \vec{P} + \frac{e}{\Omega} \sum_i n_i \vec{a}_i, \quad (1)$$

where e is the electron charge, n_i are integers, \vec{a}_i are the primitive lattice vectors, and Ω is the unit cell volume. In

the following discussion, we shall set $\Omega = 1$ such that \vec{P} can be regarded as a dipole moment per unit cell. This is a direct consequence of the translation symmetry of the lattice. Additionally, \vec{P} has to also satisfy the relevant symmetries of the crystal, which places great restriction on the allowed values of \vec{P} , thereby discretizing it. For example, in one dimension the only point group symmetry is inversion, which requires that \vec{P} and $-\vec{P}$ must be equivalent. This leads to two possibilities of \vec{P} (0 and $ea/2$),¹⁰ and a Z_2 classification. Thus here crystal symmetry discretizes polarization into two distinct classes. Each class in itself is a set of equivalent values, linked by lattice vectors due to translation symmetry. We later show that distinct classes are topologically disparate.

Next we study the impact of C_3 symmetry on the values of polarization. Let us consider a 2D lattice with C_3 rotational symmetry. We denote the two primitive lattice vectors by \vec{a} and \vec{b} . The polarization vector can be expressed as $\vec{P} = e(\alpha\vec{a} + \beta\vec{b})$. Consider the in-plane rotation \hat{R} by an angle of $2\pi/3$. \hat{R} operates on the lattice vectors such that

$$\hat{R}(\vec{a}) = \vec{b} - \vec{a}, \quad \hat{R}(\vec{b}) = -\vec{a}, \quad (2)$$

and \vec{P} transforms according to

$$\hat{R}(\vec{P}) = \vec{P}' = e[\alpha\vec{b} - (\alpha + \beta)\vec{a}]. \quad (3)$$

However, the transformed vector \vec{P}' must be equivalent to the starting value \vec{P} according to Eq. (1), i.e.,

$$\vec{P}' = \vec{P} + e(m\vec{a} + n\vec{b}). \quad (4)$$

Combining the above equations of \vec{P}' yields possible values for α and β :

$$\alpha = \frac{n-m}{3} = \frac{j}{3}, \quad \beta = -\frac{m+2n}{3} = \frac{j}{3} - n, \quad (5)$$

where n, m , and j are integers. The polarization values allowed by C_3 symmetry thus fall into three distinct classes described by 0, $e(\vec{a} + \vec{b})/3$, $2e(\vec{a} + \vec{b})/3$, and corresponding series of equivalent values given by Eq. (1).

This result has two important consequences. First, it shows that while zero is an allowed value, C_3 symmetry does not preclude nonzero polarization values, as is sometimes assumed in the literature. This misconception is a result of the classical intuition that as with forces, one can cancel polarization vectors in opposing directions. While this may apply for dipole vectors in finite, discrete charge distributions, it is not true for bulk crystalline insulators. Secondly, and more importantly, the above result suggests that 2D crystalline insulators with C_3 symmetry can be distinguished by the three distinct classes of \vec{P} , giving rise to a Z_3 classification with \vec{P} as a class index. Following the same procedure, one can verify that C_6 rotational symmetry, e.g., as seen in graphene, allows only zero polarization in insulators. Generally speaking, consider a system described by a parameter-dependent Hamiltonian $H(\lambda)$. As long as varying λ does not change the crystal symmetry, \vec{P} must remain discretized. If there is a sudden change in \vec{P} , then there must be a singularity in the phase of the Bloch functions, which signals the closing of the band gap.

III. Z_3 TOPOLOGICAL PHASE TRANSITION

We now provide a concrete example of Z_3 topological states by constructing a tight-binding model. Let us consider a honeycomb lattice with two orbitals, denoted by ϕ_α and ϕ_β , on each site. We assume that there is a nearest-neighbor hopping t between orbitals from the same type, and an on-site interorbital coupling t' between the α and β orbitals. To lower the symmetry from C_6 to C_3 , the A and B sublattices are assumed to have opposite site energies, $\pm\Delta_\alpha$ and $\pm\Delta_\beta$, for each type of orbital. The tight-binding Hamiltonian is given by

$$H = t \sum_{\langle ij \rangle} (c_{\alpha i}^\dagger c_{\alpha j} + c_{\beta i}^\dagger c_{\beta j}) + t' \sum_i (c_{\alpha i}^\dagger c_{\beta i} + c_{\beta i}^\dagger c_{\alpha i}) + \sum_i \xi_i (\Delta_\alpha c_{\alpha i}^\dagger c_{\alpha i} + \Delta_\beta c_{\beta i}^\dagger c_{\beta i}), \quad (6)$$

where $\xi_i = \pm 1$ for A and B sublattices. The corresponding Bloch Hamiltonian is obtained by Fourier transform:

$$H(\vec{k}) = \begin{pmatrix} \Delta_\alpha & tV_k & t' & 0 \\ tV_k^* & -\Delta_\alpha & 0 & t' \\ t' & 0 & \Delta_\beta & tV_k \\ 0 & t' & tV_k^* & -\Delta_\beta \end{pmatrix}, \quad (7)$$

where the structural factor V_k is given by $V_k = 1 + 2 \cos(\sqrt{3}/2k_x) \cos(k_y/2) - 2i \sin(\sqrt{3}k_x/2) \cos(k_y/2)$.

Next we show that at half-filling the system can be tuned to three topologically distinctive states by changing the parameters without breaking the C_3 symmetry. To guarantee charge neutrality, we assign an ionic charge of $2|e|$ to each lattice site. We first identify the gap closing point in the parameter space because \vec{P} cannot change unless the band gap

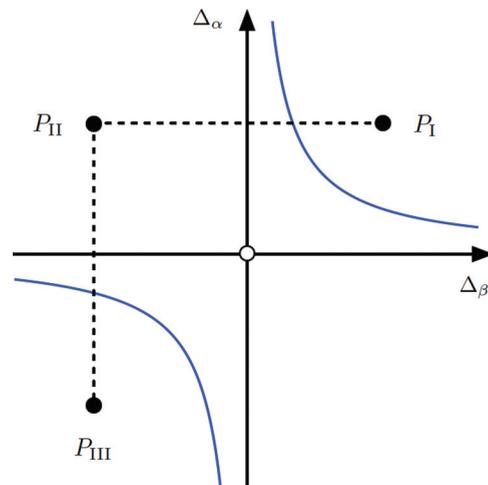


FIG. 1. (Color online) Topological phase diagram of the tight-binding model described by the Hamiltonian (7). The solid (blue) curve is the phase boundary given by $\Delta_\alpha \Delta_\beta = t^2$. In each region, the polarization is given by $P_I = -(\vec{a} + \vec{b})/3$, $P_{II} = 0$, and $P_{III} = (\vec{a} + \vec{b})/3$. The dashed line indicates a representative path in the parameter space that undergoes the topological phase transition twice.

closes. The band energies at the K point are given by

$$E = \pm(\Delta_\alpha + \Delta_\beta) \pm \sqrt{(\Delta_\alpha - \Delta_\beta)^2 + 4t'^2}. \quad (8)$$

Obviously, when $t' = \sqrt{\Delta_\alpha \Delta_\beta}$ the band gap will close, which signals a topological phase transition characterized by a sudden change of \vec{P} . To confirm this statement, we calculate the polarization at three representative points in the Δ_α - Δ_β plane, and indeed find three inequivalent values of \vec{P} predicted by Eq. (5). Note that the polarization has two contributions: the electronic and ionic contribution. Here the electronic contribution is calculated according to the Berry-phase formula,^{13,14} whereas the ionic contribution is calculated by summing over the lattice site in a unit cell. Separately, both contributions depend on the choice of origin; only the total polarization is origin-independent. The resulting topological phase diagram is shown in Fig. 1.

IV. MATERIAL REALIZATION

We now present a realistic material system, graphene on h -BN substrate,^{18–21} in which various Z_3 topological states can be realized. Specifically, we consider four cases: h -BN, AA stacking of graphene on h -BN, and AB stacking of graphene on h -BN with either boron or nitrogen atoms sitting directly underneath the carbon atom. Although graphene has C_6 rotational symmetry, placing graphene on h -BN reduces the symmetry from C_6 to C_3 , allowing nonzero polarization values to emerge.

We have performed first-principles calculations to obtain the polarization in these structures and compare with our symmetry analysis. While the carbon-carbon (C-C) bond length in graphene is known to be 1.42 Å, h -BN has a B-N bond length of 1.46 Å,²⁴ hence the mismatch is very small, $\sim 2\%$. Our initial structures were comprised, as shown in Fig. 2, of bulk monolayer h -BN and various stacking of graphene monolayer on it. We lattice-matched h -BN to graphene by taking an initial lattice constant of 1.417 Å, and we constructed supercells representing these materials in bulk (see Fig. 2). The out-of-plane distance between graphene and h -BN was taken to be 3.2 Å.¹⁸ The vacuum along the z direction was taken to be 30 Å approximately. We used the Vienna *ab initio* Simulation Package (VASP),²⁵ which uses a plane-wave basis set and employed PAW pseudopotentials,²⁶ along with a local approximation to the exchange-correlation potential (LDA).²⁷ We set an energy cutoff of 400 eV and a k -mesh of $4 \times 4 \times 1$ for the self-consistent run and $36 \times 36 \times 1$ for the subsequent polarization calculation.

The total polarization can be divided into electronic and ionic parts. While the electronic part of the polarization was calculated using the Berry phase formula,^{13,14} the ionic part was obtained from the dipole density distribution. Polarization values thus calculated for bulk structures shown in Fig. 2 are listed in Table I, in corresponding order. We list α and β for every \vec{P} , such that $\vec{P} = e(\alpha\vec{a} + \beta\vec{b})$, where \vec{a} and \vec{b} are the corresponding lattice vectors of the system. In complete agreement with our symmetry analysis, all obtained values fell into and exhausted the three topological classes predicted by Eq. (5).

Here we comment on the zero polarization found in h -BN.^{28,29} The electronic structure of h -BN can be well

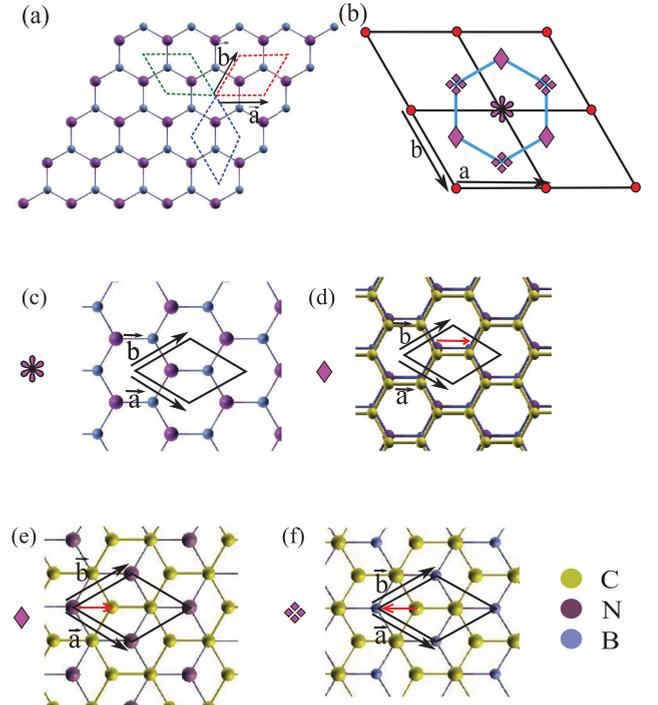


FIG. 2. (Color online) (a), (b) Schematic illustration of polarization in systems with C_3 symmetry. (a) h -BN lattice with three equivalent unit cells. (b) Possible values of polarization. Each topological class is marked by a specific symbol. Parts (c)–(f) display calculated values of polarization for different structures and the corresponding topological classes. (c) Structure 1: h -BN monolayer; (d) structure 2: AA stacking of graphene monolayer on h -BN; (e) AB stacking of graphene monolayer on h -BN with a carbon sublattice lying above the boron sublattice; and (f) structure 4: AB stacking with a carbon sublattice lying above the nitrogen sublattice. The unit cells and lattice vectors \vec{a} and \vec{b} are marked in black, whereas the polarization vector is marked in red. Colors used to represent various atoms are listed.

described by taking the ionic limit, i.e., the boron atom loses all its valence electrons to nitrogen. The nominal charges at the boron and nitrogen sites are therefore $+3$ and -3 , respectively. (One can verify that in the ionic limit, the ionic and electronic contributions agree with the DFT calculation.)

TABLE I. In-plane polarization values for the structures shown in Fig. 2, specified in terms of lattice vectors \vec{a} and \vec{b} . We tabulate the values of the ionic part \vec{P}_{ion} and the electronic part \vec{P}_{ele} , followed by the total value of polarization \vec{P} . All values are in terms of electronic charge \times lattice vector such that $\vec{P} = e(\alpha\vec{a} + \beta\vec{b})$.

System	\vec{P}_{ele}		\vec{P}_{ion}		\vec{P}	
	α ($e * \vec{a}$)	β ($e * \vec{b}$)	α ($e * \vec{a}$)	β ($e * \vec{b}$)	α ($e * \vec{a}$)	β ($e * \vec{b}$)
1	$-\frac{2}{3}$	$-\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	0	0
2	0	0	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$	$\frac{1}{3}$
3	$\frac{2}{3}$	$\frac{2}{3}$	0	0	$\frac{2}{3}$	$\frac{2}{3}$
4	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{2}{3}$	$\frac{1}{3}$	$\frac{1}{3}$

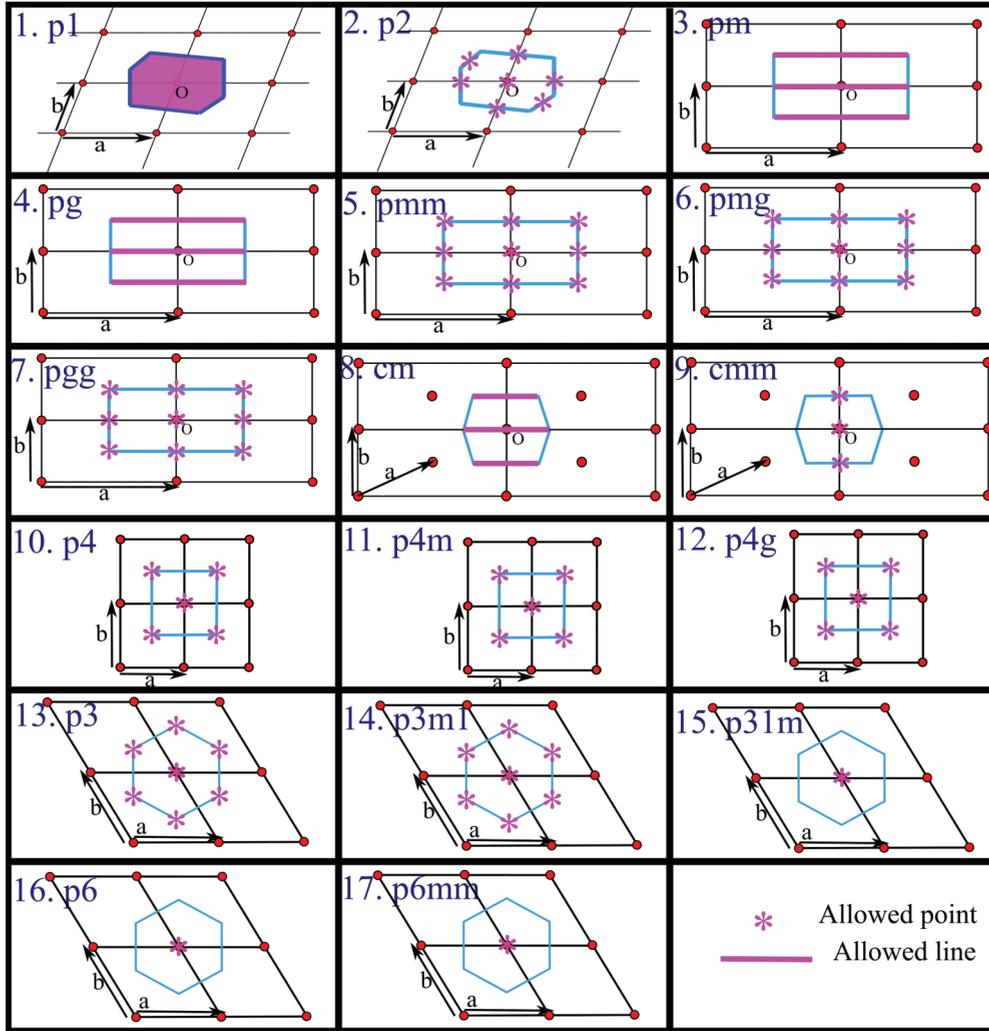


FIG. 3. (Color online) Allowed values of polarization for all 17 two-dimensional space groups. The corresponding Wigner-Seitz cells for various lattices are displayed in blue. Allowed points and lines of points are marked in magenta. Allowed values of polarization are vectors joining the origin of the Wigner-Seitz cells to the points marked.

This guarantees that the total polarization of *h*-BN will always be an integer multiple of $\vec{a} + \vec{b}$, which is equivalent to zero. If we make an artificial crystal by replacing boron and nitrogen with beryllium and oxygen, then the total polarization will not vanish. So the zero polarization of *h*-BN is not because C_3 rotational symmetry forbids other values, rather it is due to simple electron counting.

V. POLARIZATION IN 2D SPACE GROUPS

A similar analysis can be carried out for all 17 two-dimensional space groups. The allowed values of polarization derived from symmetry constraints are shown in Fig. 3.

Several remarks are in order. For space group p_1 , the allowed value of \vec{P} forms a continuum and fills up the entire Wigner-Seitz cell. This is consistent with the fact that the only point group symmetry operation of p_1 is the identity operator and there is no topological classification protected by p_1 . We also note that for several space groups, the allowed value of \vec{P} forms a line in one direction but is still quantized in the other

direction. In this situation, a topological classification can be obtained by taking the discrete component of \vec{P} .

VI. SUMMARY

We have presented polarization as a topological index protected by space group symmetry for crystalline insulators. In particular, we derive three distinct topological classes for C_3 rotational symmetric systems. Topological phase transitions between these classes are shown to be accompanied by closing the band gap. We complete the analysis by deriving polarization values for all 17 2D space groups, which provides rich possibilities of topologically distinct classes. The topological classification scheme discussed here can be readily applied to interacting systems via the many-body formulation of polarization.^{22,23}

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