A criterion of the non-existence of surface states in a semi-infinite crystal

Huiping Wang, Tingting Gao, and Ruibao Tao

State Key Laboratory of Surface Physics and Department of Physics, Fudan University, Shanghai 200433, China

(Dated: July 7, 2014)

An infinite crystal can be constructed by an infinite number of parallel two-dimensional (hkl) crystal planes coupled to each other. For crystals with negligible spin-orbit coupling, we report a rigorous proof of a criterion on the non-existence of surface states in a semi-infinite crystal with the crystal symmetry. The forward transfer to be the same as the backward one, called as F-B dynamical symmetry, is key to realize the criterion. Based on lattice model Hamiltonian with coupling between the nearest neighbor crystal planes only, we prove that a cut crystal will not be able to accommodate any surface states if the original infinite crystal has reflection symmetry about every crystal plane which results in F-B symmetry. The criterion provide a platform to simply conclude whether surface states exist or not in a cut crystal. For any such crystals, the non-existence or existence of surface states depends on the cut direction of the crystal plane. Since the spin-orbit coupling breaks the chiral symmetry, resulting in the F-B asymmetry, surface states can emerge in the (hkl) cut crystal with spin-orbit coupling.

PACS numbers:

Introduction.—Edge or surface, interface states, possessing some novel physical properties, have been attracting considerable attention. Recent decades have witnessed great interest in the study of edge or surface states for 2D or 3D crystals. Many interesting and prominent physical phenomena are tightly related to the existence of edge or surface states, such as quantum Hall effect (QHE) [1,2], quantum spin Hall effect (QSH) [3,4], topological insulator (TI) [5,6], topological superconductor (TSC) [7,11] and topological Anderson insulator (TAI) [12,15] as well as surface reconstruction of some semiconductors [19,20]. The surface reconstruction in semiconductors Si and Ge can be ascribed to the existence of surface states which provide the energy levels to be partly filled with mobile surface charges coupled with surface softened phonon modes. Gapless edge or surface states that exist in QSH and TIs come from the chiral symmetry breaking due to spin-orbit coupling (SOC), which is highly attractive in recent studies.

In this letter, we would like to focus on the majority of crystals where the SOC is unimportant and can be neglected, such as some dielectric materials like $ABO_3$ oxides, etc. For semiconductors or insulators, surface states created by cutting the surface can provide some new physical phenomenon. Especially, the electric conduction along domain walls in ferroelectric materials has attracted intense recent studies [21,22] due to the possibility of creating and controlling Nano-scale 1D/2D conductive paths in wide band gap insulators. In general, for such insulating materials with negligible SOC, different cut surface of the same crystal may show different behavior for the existence of surface states. For experimentalists, it would be very much useful if there is a criterion that can qualitatively tell which cut direction can be favorable to generate much more surface states. The criterion may demonstrate the underlying relationship between the existence or non-existence of surface states and the crystal symmetry in the absence of SOC.

In general, an infinite 3D crystal can be described by an infinite number of parallel two-dimensional crystal planes (CPs) which are periodically arranged one by one with coupling. The direction of CPs can be denoted by Miller indices (hkl), where h, k and l can be arbitrary integers. A semi-infinite crystal with the (hkl) cut surface is called the (hkl) cut crystal. In terms of a general lattice model Hamiltonian with the hopping between the nearest neighbors (n.n.) CPs, the criterion can be phrased as follows:

Criterion: A (hkl) cut crystal with negligible SOC will not allow to have any surface states if the original infinite crystal has reflection symmetry for every (hkl) crystal plane.

The criterion also covers the case of 2D crystals, then the "surface" just means the edge line (atomic chain). Although the hopping are considered for the n.n. CPs, the coupling within CPs can contain hopping to all possible neighbors, i.e., not only the nearest neighbor (n.n.) ones. In our discussion, the transfer matrix approach [23,24] is applied.

The crystals with the reflection symmetry are only one of the two types: Type I: “...P-P-P-P-...” [Fig.1a] and Type II: “...P-Q-P-Q-...” [Fig.1b] where P and Q represent CPs. The same P (Q) represents exactly the same CP and $P \neq Q$ means that $P$ and $Q$ are two different CPs. The bar “~” roughly describes the distance between the n.n. planes. The same “~” means the same distance. Since Type II “...P-Q-P-Q-...” can be dynamically transformed into Type I: “...P-P-P-...”, thus we concentrate our attention on the proof of the criterion for Type I at first and then turn back to Type II.

Proof of criterion for Type I.—For the simplest case, each CP only has single electron mode that corresponds to one atomic orbit per unit cell. Under the n.n. hopping approximation between CPs, the study of surface states...
in this case is exactly the same as that of edge states in the semi-infinite 1D single orbit atomic chain. As is well known, no edge states exist in the semi-infinite 1D atomic chain for both Type I and II when the forward hopping constant equals to the backward one [24]. Thus, we will take into account the proof of the criterion for the case where each CP $P$ contains $n (\geq 1)$ electron modes, that is, each CP contains many (and maybe different) atoms per unit cell and each atom may contribute many different atomic orbits. For a semi-infinite crystal (SIC), each CP has the periodic structure and is dimensionally lower than the original crystal. Thus, the Fourier transformation (FT) is applied to each CP since the wave vector $\mathbf{k}$ is a good quantum number. Take the diagonal representation of the Hamiltonian of each CP, then the coupling between the n.n. CPs are introduced.

For a cut crystal “P-P-P-P-P-...” in Type I [Fig.1a], it is not difficult to obtain QDEs:

$$E_{n \times n} \Psi_i = F_{n \times n} \Psi_{i+1} + B_{n \times n} \Psi_{i-1}, i \geq 1; \tag{1}$$

where $\Psi^T_i = (\psi_i^{(1)}(\mathbf{k}), \psi_i^{(2)}(\mathbf{k}), \cdots, \psi_i^{(n)}(\mathbf{k}))$ and $\{\psi_i^{(\alpha)}(\mathbf{k}) : \alpha \in \{1, 2, \cdots, n\}\}$ are the second quantized Fermi wave functions of \(\alpha\)th electron mode in the \(i\)th CP. $F_{n \times n}$ (or $B_{n \times n}$) describes the $n \times n$ forward (backward) hopping matrix from the plane $P_i$ to its n.n. plane $P_{i+1}$ ($P_{i-1}$) and $n$ can be any finite positive integers. $B_{n \times n}$ is defined as $E_{n \times n} = diag\{E_1, E_2, \cdots, E_n\}$ and $E_\alpha = E - e_\alpha(\mathbf{k}) : \alpha = 1, 2, \cdots, n$. $E$ are the energy levels of electron waves propagating in the SIC and $\{e_\alpha : \alpha = 1, 2, \cdots, n\}$ are energies of eigen-modes renormalized at each CP. The elements of $F_{n \times n}$, $B_{n \times n}$ and $\{e_\alpha : \alpha = 1, 2, \cdots, n\}$ are $\mathbf{k}$ dependent. From now on, we omit the symbol $\mathbf{k}$ for simplicity. When the original infinite crystal has the reflection symmetry for each crystal plane, then we have $F_{n \times n} = B_{n \times n} = F_{n \times n}^+$. Eq.(1) can be rewritten as

$$
\begin{cases}
E_{n \times n} \Psi_i = F_{n \times n} \Delta \Psi_i, \\
\Delta \Psi_i = \Psi_{i+1} + \Psi_{i-1},
\end{cases} \tag{2}
$$

The matrices $F_{n \times n}$ and $E_{n \times n}$ are hermitian with dimensionality $n$. Here we adopt the dimensional reduction method to reduce the dimensionality $n$ in Eq. (2) to 1. We will prove that no surface waves can accommodate in a SIC for any energy $E$. For the general case, we assume that $F_{n \times n}$ and $E_{n \times n}$ are arbitrary square matrices and not limited to hermitian matrices.

**Proof for $n \geq 3$ in Type I.**—By means of dimensional reduction method, we will reduce the dimensionality $n$ in Eq.(2) into 1 or 2. Let us first consider an energy such that $E : \det(E_{n \times n}) \neq 0$. Since $\det(E_{n \times n}) \neq 0$, we can obtain from Eq.(2)

$$\Psi_i = (E_{n \times n}^{-1} F_{n \times n}) \Delta \Psi_i, i \geq 1. \tag{3}$$

It is well known that a square matrix $(E_{n \times n}^{-1} F_{n \times n})$ can be decomposed into a Jordan matrix via a similarity transformation $J_{n \times n} = U_{n \times n}^{-1}(E_{n \times n}^{-1} F_{n \times n}) U_{n \times n}$. $J_{n \times n}$ is a block diagonal matrix: $J_{n \times n} = \sum_{i=1}^{s} J_i(\lambda_i)$ where

$$J_i(\lambda_i) = \begin{pmatrix} \lambda_i & c_i & 0 & 0 \\ 0 & \lambda_i & \cdots & 0 \\ 0 & 0 & \cdots & c_i \\ 0 & 0 & 0 & \lambda_i \end{pmatrix}, c_i \neq 0 \text{ or } c_i = 0,$$

and $\{\lambda_i : i = 1, 2, \cdots, s\}$ in $J_{n \times n}$ are eigenvalues of the matrix $(E_{n \times n}^{-1} F_{n \times n})$. Now we have

$$\Psi_i = J_{n \times n} \Delta \Psi_i', \Psi_i' = U_{n \times n}^{-1} \Psi_i, \Psi_0' = 0. \tag{4}$$

In terms of the lowest-right-most element of the Jordan matrix $J_{n \times n}$, the first equation can be reached immediately for $\psi_i^{(n)}$

$$\psi_i^{(n)} = \lambda_s \Delta \psi_i^{(n)}. \tag{5}$$

Eq.(5) is exactly the same as the transfer matrix equation of 1D atom chain with single electron mode. It has been known that there is no edge states for any energy $E$ no matter whether $\lambda_s = 0$ or $\lambda_s \neq 0$ [24]. Thus we arrive at $\{\psi_i^{(n)} = 0 : i \geq 1\}$ for the solution of surface states. After back-substituting $\{\psi_i^{(n)} = 0 : i \geq 1\}$ into Eq.(4), we find that surface states are also impermissible for the $(n-1)^{th}$ mode, yielding $\{\psi_i^{(n-1)} = 0 : i \geq 1\}$. After step by step, we obtain trivial solutions of all surface waves: $\{\psi_i' = 0 : i \geq 1\}$ that results in $\Psi_i' = U_{n \times n} \Psi_i' = 0$. Hence no surface states are allowed for $\det(E_{n \times n}) \neq 0$.

Next let us think over some energies $E$ such that $\det(E_{n \times n}) = 0$. Now we apply a Jordan transformation $V_{n \times n}$ to the square matrix $E_{n \times n} = E_{n \times n}$.
\[V_{n \times n}^{-1} E_{n \times n} V_{n \times n} \text{ and have}
\]
\[E_{n \times n}^f \Psi_i = F_{n \times n} \Delta \Psi_i, \Psi_i = V_{n \times n}^{-1} \Psi_i, \Psi_0 = 0, i \geq 1, \quad (6)
\]
here \(F_{n \times n} = V_{n \times n}^{-1} E_{n \times n} V_{n \times n} \). \(E_{n \times n}^f = \sum_{i=1}^{m} J_i(\lambda_i)\) where we have arranged such that the sub-matrix \(J_1\) contains \(\lambda_1 = 0\). Without loss of generality, we can assume the first block is a two-order Jordan sub-matrix at first. For other cases where \(J_1(\lambda_1 = 0)\) is one or greater than two, we can do similar demonstration as we do for a two-order Jordan block \(J_1(\lambda_1 = 0)\). The derivation can proceed by considering two scenarios: 1) Suppose \(F_{11}^f \neq 0\). We can obtain from the first row of Eq.(6),
\[\Delta \psi_i^{(1)r} = -\frac{1}{F_{11}^f} \sum_{\alpha=2}^{n} F_{1\alpha}^f \Delta \psi_i^{(\alpha)r} + c_1 \psi_i^{(2)r} : i \geq 1. \quad (7)
\]
Substituting Eq.(7) into Eq.(6), we can arrive at
\[E_{(n-1) \times (n-1)} (n-1) \psi_i = F_{(n-1) \times (n-1)} (n-1) \Delta \Psi_i, \quad (8)
\]
here \(\Delta \psi_i = (\psi_i^{(2)}), (\psi_i^{(3)}), \ldots, (\psi_i^{(n)})\) and \(\{ F_{\alpha \beta}^{(n-1)} = F_{\alpha \beta} - F_{\alpha 1}^f F_{1 \beta} / F_{11}^f \} \). Thus, we have reduced the dimensionality \(n\) in Eq.(6) into \(n - 1\).

2) Next suppose \(F_{11}^f = 0\): Now we focus on the 1st column matrix elements of \(F_{n \times n}\). If all of \(\{ F_{1j}^f : j = 1, 2, \ldots, n \}\) are zero, the reduction of the dimensionality in Eq.(6) is already reached. Thus, we assume \(\{ F_{\beta \beta}^f \neq 0 : \beta \in \{2, 3, \ldots, n\}\) without loss of generality and obtain
\[\Delta \psi_i^{(1)r} = -\frac{1}{F_{\beta 1}^f} \sum_{j=2}^{n} F_{\beta j}^f \Delta \psi_i^{(j)r} - \lambda_i \psi_i^{(\beta)r} - c_2 \psi_i^{(\beta+1)r}. \quad (9)
\]
After plugging the above equation into Eq.(6), we can get
\[\Theta_{(n-1) \times (n-1)} \psi_i = F_{(n-1) \times (n-1)} (n-1) \Delta \Psi_i, i \geq 1, \quad (9)
\]
here \(\gamma \in \{1, 2, \ldots, s\}\), \(\{ F_{ij}^f = F_{j1}^f - F_{11}^f \Delta \psi_i^{(j)} / F_{11}^f \} \) and \(\Delta \psi_i = (\psi_i^{(2)}, \psi_i^{(3)}, \ldots, (\psi_i^{(n)})\). Elements in the matrix \(\Theta_{(n-1) \times (n-1)}\) are functions of \(\{ E_{\alpha} : \alpha = 1, 2, \ldots, n\}\) and hopping constants. \(F_{(n-1) \times (n-1)}\) is a renormalized hopping matrix, dependent on the energy \(E\). As a result, the dimensionality \(n\) in Eq.(6) has been reduced to \(n - 1\). If the determinant of \(E_{(n-1) \times (n-1)}\) or \(\Theta_{(n-1) \times (n-1)}\) is zero, we will continue to reduce the dimensionality \(n - 1\) in Eq.(8) or/and Eq.(9) to \(n - 2\) by following the similar steps from Eq.(6) to Eq.(9). If necessary, we can do more reductions similar to above and eventually reduce the dimensionality in Eq.(6) to 1 or 2. Meanwhile, it is easy to see that other modes \(\{ \Delta \psi_i^{(l)} : l = 2, 3, \ldots, n \text{ or } l = 3, 4, \ldots, n \}\) are either the linear combinations of \(\{ \psi_i^{(j)}, \Delta \psi_i^{(j)} : j = 1 \text{ (or } j = 1, 2\}\) or can be decoupled as local modes when the dimensionality in Eq.(6) is reduced to 1(2). No surface states exist for the dimensionality 1 (as well known) when the forward hopping constant is equal to the backward hopping one, neither for the dimensionality 2, as will be proved in the following.

**Proof for \(n = 2\) in Type I.**—When \(n = 2\), Eq.(2) is rewritten as
\[E_{2 \times 2} \Psi_i = F_{2 \times 2} \Delta \Psi_i, \Psi_0 = 0, i \geq 1, \quad (10)
\]
here \(\Psi_i^T = (\psi_i^{(1)}, \psi_i^{(2)})\) and assuming \(E_{2 \times 2}\) and \(F_{2 \times 2}\) are general matrices in order to cover the previous case where the dimensionality in Eq.(6) is reduced to 2 when \(n \geq 3\) and \(\det(E_{n \times n}) = 0\). To ensure the proof valid for any energy \(E\) and any crystal structures, we must discuss all possible matrix structures of \(E_{2 \times 2}\) and \(F_{2 \times 2}\).

At first, note that when \(\det(E_{2 \times 2}) \neq 0\) or \(\det(F_{2 \times 2}) \neq 0\), we obtain \(\{ \psi_i^{(1)} = 0, \psi_i^{(2)} = 0 : i \geq 1\}\) for surface waves by following the similar steps from Eq.(3) to Eq.(5).

Next, think over the special case where \(\det(E_{2 \times 2}) = 0\) and \(\det(F_{2 \times 2}) = 0\). We apply a Jordan similar transformation \(U_{2 \times 2}\) for \(E_{2 \times 2}\), then Eq.(10) can be written as
\[
\begin{cases}
J_{2 \times 2}^f \Psi_i^f = F'_{2 \times 2} \Delta \Psi_i, \Psi_i^f = U_{2 \times 2}^{-1} \Psi_i,
J_{2 \times 2}^f = U_{2 \times 2}^{-1} E_{2 \times 2} U_{2 \times 2} = \begin{pmatrix} \lambda_1 & c_0 \\ 0 & 0 \end{pmatrix},
\end{cases}
\quad (11)
\]
here \(F_{2 \times 2} = U_{2 \times 2}^{-1} F_{2 \times 2} U_{2 \times 2}\) and \(\{\lambda_1, c_0\}\) can be zero or nonzero. We further examine the following three possible situations:

i) \(c_0 = 0\) and \(\lambda_1 = 0\)

We can apply the Jordan transformation again to \(F'_{2 \times 2}\) and since \(\det(F_{2 \times 2}) = \det(F'_{2 \times 2}) = 0\), Eq.(11) becomes
\[
\begin{cases}
0_{2 \times 2} = J'_{2 \times 2} \Delta \Psi_i', \Delta \Psi_i' = W_{2 \times 2}^{-1} \Delta \Psi_i',
J'_{2 \times 2} = W_{2 \times 2}^{-1} F'_{2 \times 2} W_{2 \times 2} = \begin{pmatrix} \alpha_1 & c_1 \\ 0 & 0 \end{pmatrix},
\end{cases}
\quad (12)
\]
When \(\alpha_1 = 0\) and \(c_1 = 0\), \(\{ \Delta \psi_i^{(1)}, \Delta \psi_i^{(2)}\}\) fully decouple and become local modes within each CP. When \(\alpha_1 \neq 0\) and \(c_1 = 0\), \(\Delta \psi_i^{(1)} = 0\) corresponds to an extended mode and \(\Delta \psi_i^{(2)}\) is decoupled as the local mode.

When \(\alpha_1 = 0\) and \(c_1 \neq 0\), \(\Delta \psi_i^{(2)} = 0\) means the nonexistence of surface states and \(\Delta \psi_i^{(1)}\) becomes the local modes without propagation among the CPs.

ii) \(c_0 \neq 0\) and \(\lambda_1 = 0\)

At first, we note that when \(F'_{21} \neq 0\) or \(F'_{22} \neq 0\), \(\psi_i^{(1)}\) and \(\psi_i^{(2)}\) become local modes within each CP or are zero solutions for surface states.

Next, consider the special case where \(F'_{21} = 0\) and
$F'_{22} = 0$, then we get from Eq.(11)

$$c_0\psi^{(2)e}_i = F'_{11}\Delta\psi^{(1)e}_i + F'_{12}\Delta\psi^{(2)e}_i.$$  

(13)

When $F'_{11} = 0$, Eq.(13) turns into $c_0\psi^{(2)e}_i = F'_{12}\Delta\psi^{(2)e}_i$ and we obtain \{\psi^{(2)e}_i = 0 : i \geq 1\} for surface states. When $F'_{11} \neq 0$, \{\psi^{(1)e}_i, \psi^{(2)e}_i\} are coupled together. If there are surface states existing for \{\psi^{(1)e}_i, \psi^{(2)e}_i\}, we can have $\Delta\psi^{(1)e}_i = \beta \Delta\psi^{(2)e}_i$ where $\beta$ is a non-zero constant.

Then Eq. (13) becomes $c_0\psi^{(2)e}_i = (F'_{11} + F'_{12})\Delta\psi^{(2)e}_i$ that results in \{\psi^{(2)e}_i = 0 : i \geq 1\} for surface modes, leading to \{\psi^{(1)e}_i = 0 : i \geq 1\}. Therefore, no surface states can exist in the SIC.

i) $c_0 = 0$ and $\lambda_1 \neq 0$

The proof is almost exactly similar to the case \{c_0 \neq 0 and $\lambda_1 = 0\} and we get the same conclusion.

Up to now, the criterion has been analytically proved for the cut crystals with \textquotedblleft Q-Q-Q-Q-\ldots\textquotedblright by means of dimensional reduction method.

**Proof of criterion for Type II.**—In Type II, the crystal has two different CPs: $P$ and $Q$. We just discuss the $Q$ cut crystal \textquotedblleft Q-P-Q-P-\ldots\textquotedblright [Fig.1b] since the discussion for $P$ cut crystal will be similar. Now the QDEs for the $Q$ cut crystal are

$$\begin{cases}
E^{(P)}_{n \times m} \Psi_i = F_{n \times x} (\Phi_i + \Phi_{i+1}), \\
E^{(Q)}_{m \times m} \Phi_i = (F_{n \times m})^+ (\Psi_{i-1} + \Psi_i), \ i \geq 1,
\end{cases}$$  

(14)

here the boundary conditions are $\Phi_0 = 0_{n \times 1}$ and $\Psi_0 = 0_{n \times 1}$ and the CP $P$ has $n$ modes and $Q$ has $m$ ones. $n$ and $m$ can be equal or unequal. \{$E^{(P)}_{n \times m}, E^{(Q)}_{m \times m}\} are defined as $E^{(P)}_{n \times m} = diag\{E^{(P)}_1, E^{(P)}_2, \ldots, E^{(P)}_n\}$, $E^{(Q)}_{m \times m} = E - \omega^2_0$, $i = 1, 2, \ldots, \lambda_1$ and $\lambda_P = n (m)$ when $\alpha = P (Q)$. After some simple calculations, Eq.(14) can be rewritten as

$$\begin{cases}
E^{(P)}_{(n+m) \times (n+m)} \Pi_i = F^{(P)}_{(n+m) \times (n+m)} \Delta \Pi_i, \\
E^{(Q)}_{(m \times m)} = \begin{pmatrix}
2F_{n \times m} & -2F_{n \times m} \\
-2F_{n \times m} & E^{(Q)}_{m \times m}
\end{pmatrix}, \\
F_{(n+m) \times (n+m)} = \begin{pmatrix}
0_{n \times n} & 0_{n \times m} \\
F_{n \times m} & 0_{m \times m}
\end{pmatrix}, \Pi_i = \begin{pmatrix}
\Psi_i \\
\Phi_i
\end{pmatrix},
\end{cases}$$

here $\Phi_i = \Phi_{i+1} + \Phi_i$ and $\Delta \Pi_i = \Pi_{i-1} + \Pi_{i+1}$. Now the $Q$ cut crystal \textquotedblleft Q-P-Q-P-\ldots\textquotedblright in Type II is equivalent to the structure \textquotedblleft Q-Q-Q-Q-\ldots\textquotedblright in Type I with the dimensionality $n + m$. We can readily find \{$\Pi_i = 0$ : $\Phi_i = 0, \Psi_i = 0, i \geq 1\} for surface waves. \{$\Phi_i = 0 : i \geq 1\} yields \{$\Phi_{i+1} + \Phi_i = 0 : i \geq 1\} that leads to \{$\Phi_i = 0 : i \geq 1\}. Hence the criterion is also valid for Type II. So far, we have completed the proof of the criterion of the non-existence of surface states in the cut crystals for Type I \textquotedblleft \ ... P-P-P-\ldots\textquotedblright and Type II \textquotedblleft \ ... P-Q-P-Q-\ldots\textquotedblright.

From the demonstration above, we clearly know that

$F_{n \times n} = B_{n \times n}$ is the key point for the non-existence of surface states in the cut crystal. Other crystal structures, like \textquotedblleft \ldots P-Q-P-Q-\ldots\textquotedblright, \textquotedblleft \ldots P-P-P-P-\ldots\textquotedblright, \textquotedblleft \ldots P-Q-S-P-Q-S-\ldots\textquotedblright, etc. do break the reflection symmetry (F-B symmetry) in the above criterion, thus surface states can emerge in the SIC and can contribute some surface bands in the bulk band gap.

In application of the criterion, we can easily check the armchair edged graphene does not have edge states, since it has \textquotedblleft P-P-P-\ldots\textquotedblright structure. The conclusion is consistent with previous theoretical analysis. However, the type structure of zigzag edged graphene is \textquotedblleft P-P-P-\ldots\textquotedblright, where the F-B symmetry is broken, thus it is in favor of the existence of edge states according to our criterion. From structure symmetry analysis of Perovskite structure $ABO_3$ materials such as $PbTiO_3$ in different phases, we can easily conclude that the c-cut $ABO_3$ materials in the para-electric phase and with the polarization normal to c-axis have no surface states since their structures are the \textquotedblleft P-Q-P-Q-\ldots\textquotedblright type and but the c-cut $ABO_3$ materials with the polarization along the c-axis favor surface states due to the reflection asymmetry.[Fig.2a] Furthermore for hexagonal structure c-cut ferroelectric $YMnO_3$[Fig.2b], it have surface states due to the F-B asymmetry, consistent with the previous analysis. The conclusions of previous theoretical works can be readily qualitatively understood from the criterion.

**Conclusion.**—We have rigorously proved a criterion on the non-existence of surface states in a (hkl) cut crystal: there will not be any surface states if the original infinite crystal has reflection symmetry about every (hkl) crystal plane. In our demonstration, The longer range hopping among CPs has not been considered and the many body correlation is been neglected. Note the reflection symmetry is just a sufficient condition for the non-existence of surface states in a cut crystal. In fact, the F-B dynamical symmetry ($F_{n \times n} = B_{n \times n}$) is key to realize the criterion. The F-B symmetry is more general and can be
also applicable to other structure crystals. For crystals with negligible SOC, one can find that different cut surface of the same crystals may have different behavior for the existence of surface states. While for crystals with SOC, such as topological insulators, they break the chiral symmetry, resulting in the F-B asymmetry, thus surface states can emerge. Moreover, the criterion can be extended to $F_{n \times n} = e^{i\delta} B_{n \times n}$ where $\delta$ is a $\vec{k}$-dependent or zero. Much more detailed investigations are underway for the longer rang hopping among CPs. We hope the theoretical predication from our criterion will be helpful to determine which cut direction of the crystals is in favor of generating surface modes in new materials.

We gratefully acknowledge Professors Zhi-Xun Shen, Keji Lai, Tao Xiang, Xi Dai, Zhong Fang and Yongliang Yang for helpful discussions. The work is supported by the National Basic Research Program of China (973 Program) under the grant No.2011CB921803 and the National Natural Science Foundation of China through the grant No.11147001.

* Corresponding author: rbtao@fudan.edu.cn

[1] D. J. Thouless, M. Kohmoto, M. P. Nightingale, and M. den Nijs, Phys. Rev. Lett. 49, 405 (1982).
[2] F. D. M. Haldane, Phys. Rev. Lett. 61, 2015 (1988).
[3] C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 146802 (2005); C. L. Kane and E. J. Mele, Phys. Rev. Lett. 95, 226801 (2005).
[4] B. A. Bernevig, T. L. Hughes, and S. C. Zhang, Science 314, 1757 (2006).
[5] C. X. Liu, T. L. Hughes, X. L. Qi, K. Wang, and S. C. Zhang, Phys. Rev. Lett. 100, 236601 (2008).
[6] L. Fu, C. L. Kane, and E. J. Mele, Phys. Rev. Lett. 98, 106803 (2007); L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008).
[7] D. Hsieh et al. Nature 452, 970 (2008).
[8] H. Zhang, C. X. Liu, X. L. Qi, X. Dai, Z. Fang, and S. C. Zhang, Nat. Phys. 5, 438 (2009).
[9] Y. L. Chen et al., Science 325, 178 (2009).
[10] M. Z. Hasan and C. L. Kane, Rev. Mod. Phys. 82, 3045 (2010).
[11] X. L. Qi and S. C. Zhang, Rev. Mod. Phys. 83, 1057 (2011).
[12] L. Fu and C. L. Kane, Phys. Rev. Lett. 100, 096407 (2008).
[13] X. -L. Qi, T. L. Hughes, S. Raghu, and S. -C. Zhang, Phys. Rev. Lett. 102, 187001 (2009); X.-L. Qi, T. L. Hughes, and S. C. Zhang, Phys. Rev. B 82, 184516 (2010).
[14] A. Das, Y. Ronen, Y. Most, Y. Oreg, M. Heiblum, and H. Shtrikman, Nat. Phys. 8, 887 (2012).
[15] S. Deng, L. Viola, and G. Ortiz, Phys. Rev. Lett. 108, 036803 (2012); S. Deng, G. Ortiz, A. Poudel, L. Viola, Phys. Rev. B 89, 140507(R) (2014).
[16] J. Li, R. L. Chu, J. K. Jain, and S. Q. Shen, Phys. Rev. Lett. 102, 136806 (2009).
[17] W. Li, J. Zang, and Y. Jiang, Phys. Rev. B 84, 033409 (2011).
[18] Y. Y. Zhang, R. L. Chu, F. C. Zhang, and S. Q. Shen, Phys. Rev. B 85, 035107 (2012).
[19] J. E. Northrup and M. L. Cohen, Phys. Rev. Lett. 57, 154 (1986).
[20] W. C. Fan and A. Ignatiev, Phys. Rev. B 40, 5479 (1989).
[21] J. Seidel, et al., Nat. Mater. 8, 229 (2009).
[22] D. Meier, et al., Nat. Mater. 11, 284 (2012).
[23] D. H. Lee and J. D. Joannopoulos, Phys. Rev. B 23, 4988 (1981).
[24] Y. Y. Zhao, W. Li, and R. B. Tao, Chin. Phys. B 21, 027302 (2012).
[25] Y. Y. Zhao, W. Li, and R. B. Tao, Physica. B 407, 724 (2012).
[26] W. Ho, S. L. Cunningham, W. H. Weinberg, and L. Dobrzynski, Phys. Rev. B 12, 3027 (1975).
[27] M. Mostoller and A. K. Rajagopal, Phys. Rev. B 25, 6168 (1982).