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Magnetic instability on the surface of topological insulators

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Gapless surface states that are protected by time-reversal symmetry and charge conservation are among the manifestations of three-dimensional topological insulators. In this work we study how electron-electron interaction may lead to spontaneous breaking of time-reversal symmetry on surfaces of such insulators. We find that a critical interaction strength exists above which the surface is unstable with respect to the spontaneous formation of magnetization, and we study the dependence of this critical interaction strength on temperature and chemical potential.

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Topological states of matter are one of the main themes of modern condensed-matter physics. A recent important discovery in this field are topological insulators.[1–3] In three dimensions topological insulators are electronic materials that have a bulk gap like an ordinary insulator, but have conducting states on their surface.[1,4] The gapless spectrum on the surface arises from the topologically nontrivial band structure.[5,6] It is composed of an odd number of Dirac cones in the Brillouin zone of the two-dimensional surface. These Dirac cones cannot be gapped as long as time-reversal symmetry and charge conservation are maintained.

In this work we explore the conditions under which the surface of a strong topological insulator may lower its energy by a spontaneous breaking of time-reversal symmetry through the formation of a uniform spin polarization. The way energy may be saved by spin polarization is most easily understood for the case where there is one Dirac cone on each surface, and the chemical potential lies at the Dirac point. For such a case, two sources for energy gain may be identified. First, if the spin polarization introduces a mass term to the Dirac Hamiltonian, the filled electronic states are lowered in energy, while the energy of the unfilled states is raised. Second, as is usual for electrons, if all spins are polarized, two electrons cannot reside at the same point, and the short-distance energy cost is reduced. This is not the case in the absence of magnetization. Even though the half-filled Dirac cone includes just one electron for every momentum state, the variation of the spin's direction with that of the momentum leads to a nonzero probability of two electrons being at the same point and thus to a gain of interaction exchange energy by spin polarization.

In our analysis, carried out within the Hartree-Fock approximation, we find that there is a critical interaction strength above which the spin-polarized ground state is favorable in energy compared to the noninteracting ground state. We find this to be the case for every value of the chemical potential, for all temperatures much smaller than the bulk energy gap, and for both contact interaction and Coulomb interaction. Of the possible spin polarizations we find that the lowest energy corresponds to an out-of-plane polarization, which introduces an energy gap to the Dirac cone at the Dirac point. For contact interaction, we find the phase transition from the unpolarized to the polarized phase to be of second order both as a function of interaction strength and as a function of temperature. Finally, we find the energy gap to rise sharply as temperature is lowered below the temperature T_c of the phase transition, and it reaches values comparable to T_c at about $T \approx 0.9T_c$. We note that a gapped Dirac cone was recently observed by angle-resolved photo emission (ARPES) in the topological insulator phase,[7] but the information available is not sufficient to judge whether this observation is related to the mechanism we study.

We start with the noninteracting Hamiltonian. ARPES measurements carried out on two topological insulators, Bi_2Te_3 and Bi_2Se_3, have found that while near the Dirac point the spectrum is Dirac-like, a hexagonal warping of the Fermi surface occurs away from the Dirac point.[8–10] This phenomenon was modeled by Fu,[11] who suggested an effective Bloch Hamiltonian of the surface including a cubic term:

$$\mathcal{H}(\boldsymbol{k}) = v_0(k_x\sigma_y - k_y\sigma_x) + \lambda k^3 \cos(3\theta)\sigma_z, \tag{1}$$

where v_0 is the electron velocity near the Dirac point, λ is the warping parameter, and σ are the Pauli matrices. The above spectrum contains two branches that meet at the Dirac point. This Hamiltonian is time-reversal symmetric. At the time-reversal invariant point $k = 0$, the spectrum is degenerate and the degeneracy is protected by the time-reversal symmetry.

The interaction part of the Hamiltonian is

$$\mathcal{H}_{\mathcal{I}} = \int d\boldsymbol{r}\, d\boldsymbol{r}'\psi^{\dagger}_{\sigma}(\boldsymbol{r})\psi_{\sigma}(\boldsymbol{r})V(\boldsymbol{r}-\boldsymbol{r}')\psi^{\dagger}_{\sigma'}(\boldsymbol{r}')\psi_{\sigma'}(\boldsymbol{r}'). \tag{2}$$

Here $\psi^{\dagger}_{\sigma}(\boldsymbol{r})$ is the creation operator of an electron at point $\boldsymbol{r}$ and spin σ. We will assume that the following operator has a nonvanishing expectation value:

$$\langle\psi^{\dagger}_{\sigma}(\boldsymbol{r})\psi_{\sigma'}(\boldsymbol{r}')\rangle \equiv M_{\sigma,\sigma'}(\boldsymbol{r}-\boldsymbol{r}'). \tag{3}$$

Strictly speaking, we can interpret M as the magnetization only when $\boldsymbol{r} = \boldsymbol{r}'$. However, the expectation value (3) breaks time-reversal symmetry even when $\boldsymbol{r} \neq \boldsymbol{r}'$. We confine ourselves to uniform states, in which M will depend only on $\boldsymbol{R} \equiv \boldsymbol{r} - \boldsymbol{r}'$. This case is most relevant when the Fermi energy is located at the vicinity of the Dirac point, otherwise spin-density-wave formation is an interesting possibility.

The expectation value (3) may be written in a matrix form as $M_{\sigma,\sigma'}(\boldsymbol{r}-\boldsymbol{r}') = M_0(\boldsymbol{R})I + \vec{M}(\boldsymbol{R})\cdot\vec{\sigma}$, but since we are interested only in the spin part of the interaction and in particular the out-of-plane spin (z direction), we will assume that only $M_z \neq 0$; hence, $M_{\sigma,\sigma'}(\boldsymbol{r}-\boldsymbol{r}') \equiv M(\boldsymbol{R})\sigma_z$. In-plane magnetization will be discussed in a later part of the paper.

By denoting $F_{\boldsymbol{k}} = \int d\boldsymbol{R}\ V(\boldsymbol{R}) M(\boldsymbol{R}) \exp(-i\boldsymbol{k}\cdot\boldsymbol{R})$, we can write the mean-field Hamiltonian as

$$H^{\mathrm{MF}} \equiv \int d\boldsymbol{R}\, V(\boldsymbol{R}) M^2(\boldsymbol{R}) + \int \frac{d\boldsymbol{k}}{(2\pi)^2} c_{\boldsymbol{k}}^{\dagger} \hat{h}(\boldsymbol{k}) c_{\boldsymbol{k}}, \tag{4}$$

where

$$\hat{h} = v_0(k_x\sigma_y - k_y\sigma_x) + (\lambda k^3 \cos 3\theta - 2F_{\boldsymbol{k}})\sigma_z.$$

For a self-consistent determination of the out-of-plane magnetization, we denote the eigenvalues and the corresponding eigenstates of $\hat{h}$ as $\epsilon_{\pm}(\boldsymbol{k})$ and $(\chi_{\uparrow},\chi_{\downarrow})_{\pm}$, respectively. The $\pm$ signs refer to the positive and negative energy states. Hence, the magnetization per unit volume is

$$m = \frac{1}{\Omega}\sum_{\boldsymbol{k}} (\langle\sigma_{z-}\rangle f_{\epsilon_-} + \langle\sigma_{z+}\rangle f_{\epsilon_+}), \tag{5}$$

where

$$\langle\sigma_{z\pm}\rangle = |\chi_{\uparrow}|_{\pm}^2 - |\chi_{\downarrow}|_{\pm}^2,$$

and f_{ϵ} is the Fermi-Dirac function at energy ϵ. The trivial solution ($m = 0$) always exists, but we are interested in nontrivial solutions of this equation. The total energy per unit volume is

$$E_m = \int d\boldsymbol{R}\, V(\boldsymbol{R}) M^2(\boldsymbol{R}) + \frac{1}{\Omega}\sum_{\boldsymbol{k}} (\epsilon_- f_{\epsilon_-} + \epsilon_+ f_{\epsilon_+}). \tag{6}$$

We will define the energy cost to have finite magnetization as $\Delta E = E_m - E_0$. If we find a nontrivial solution to Eq. (5) that minimizes E_m (gives $\Delta E < 0$), we will conclude that the system forms spontaneous surface magnetization.

It is hard to determine the exact validity conditions for this variational procedure and to estimate its accuracy. Considering the effect of quantum fluctuations is beyond the scope of this paper. However, since Eq. (1) has no spin-rotational symmetry, the only symmetry that the magnetic ground state breaks is a discrete one (time reversal), hence the influence of fluctuations is suppressed. Moreover, since the procedure above relies on the existence of a bulk gap, it is clear that it requires the interaction energy to be smaller than the bulk gap. We will consider the condition $U_c < \Delta_{\mathrm{bulk}}$ as necessary for the above procedure (where U_c is the critical interaction energy and Δ_{bulk} is the bulk energy gap).

It is simplest to analyze a contact interaction, $V(\boldsymbol{R}) = \frac{g}{2}\delta(\boldsymbol{R})$. At zero temperature Eq. (5) for the magnetization $M(\boldsymbol{0}) \equiv m$ becomes

$$m = \int_{k_F} \frac{d\boldsymbol{k}}{(2\pi)^2} \frac{gm - \lambda k^3 \cos 3\theta}{\sqrt{v_0^2 k^2 + (gm - \lambda k^3 \cos 3\theta)^2}}, \tag{7}$$

where $d\boldsymbol{k} = k\,dk\,d\theta$ and k_{F} is the Fermi momentum, which is the solution to $(v_0 k_{\mathrm{F}})^2 + (\lambda k_{\mathrm{F}}^3 \cos 3\theta)^2 = \mu^2$, with μ the chemical potential. For $|\mu| < (v_0^3/\lambda)^{1/2}$, $k_{\mathrm{F}} \approx |\mu|/v_0$ is a good approximation. In general the integration has an upper cutoff in momentum, k_{Λ}, which corresponds to the momentum at which the surface states merge with the three-dimensional bands. For $\lambda = 0$ all results depend linearly on this cutoff, but for $\lambda \neq 0$ we can identify a momentum scale $q_0 \equiv (\frac{v_0}{\lambda})^{1/2}$ above which the integrand decays as k^{-3}. The cutoff dependence then disappears for $k_{\Lambda} \gg q_0$.

We find that there is a critical interaction strength g_c at which a second-order phase transition occurs, such that for $g > g_c$ there is an $m \neq 0$ solution to Eq. (7) with $\Delta E < 0$. The critical interaction strength is

$$g_c = \frac{\sqrt{\lambda v_0}}{Y(p_{\Lambda}) - Y(p_F)} = \frac{g_c(\mu = 0)}{1 - \frac{Y(p_F)}{Y(p_{\Lambda})}}, \tag{8}$$

where $p_{\Lambda,F} = k_{\Lambda,F}\sqrt{\frac{\lambda}{v_0}}$ is a dimensionless parameter and the function Y is defined by

$$Y(p) = \int_0^p \frac{p'dp'}{(2\pi)^2} \int_0^{2\pi} d\theta \frac{p'^2}{[p'^2 + (p'^3\cos 3\theta)^2]^{3/2}}. \tag{9}$$

The function $Y(p_{\Lambda})$ is a continuous, positive, and monotonically increasing function of p_{Λ} with the following asymptotic behavior:

$$Y(p_{\Lambda}) \sim \begin{cases} \frac{p_{\Lambda}}{2\pi}, & p_{\Lambda} \ll 1 \\ 0.247, & p_{\Lambda} \gg 1. \end{cases} \tag{10}$$

For $\mu = 0$ and $\lambda \to 0$, Eq. (8) becomes $g_c = 2\pi\frac{v_0}{k_{\Lambda}}$; while for $k_{\Lambda} \gg (\frac{v_0}{\lambda})^{1/2}$, Eq. (8) becomes $g_c \approx 4.1\sqrt{v_0\lambda}$. The resulting phase diagram ($\mu = 0$) in the large cutoff limit is presented in Fig. 1. Clearly, in order to get closer to a magnetic instability we need a large k_{Λ} (a large bulk energy gap) and a small Fermi velocity.

As opposed to the standard parabolic Hamiltonians with contact interaction, here the critical interaction strength g_c increases as $|\mu|$ increases. While the standard Stoner instability[12] is a Fermi-surface process where the spin-degenerate Fermi surface splits into two, in the Dirac-cone case there is no spin degeneracy and the Fermi surface remains unchanged when uniform magnetization occurs. This transition involves the entire Fermi sea.

In the limit $\lambda \to 0$, Eq. (8) gets a simple form:

$$g_c(\mu) = g_c(\mu = 0)\frac{1}{1 - \frac{k_F}{k_{\Lambda}}}. \tag{11}$$

As expected for $k_{\mathrm{F}} \to k_{\Lambda}$ (full band) magnetization formation is not possible. We note, however, that as long as the chemical potential is far from the bulk bands its effect on g_c is rather weak.

For $g \sim g_c$ we can estimate the interaction energy per particle by noticing that $\langle\mathcal{H}_{\mathcal{I}}\rangle_{\text{per-particle}} = \frac{gn_e}{8}$, where n_e is the

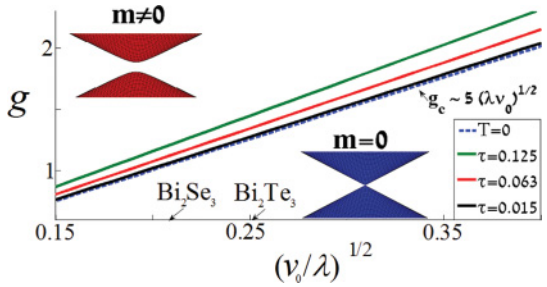

FIG. 1. (Color online) Phase diagram ($p_{\Lambda} = 2$) for contact interaction at zero (dashed line) and finite temperatures, where $\tau \equiv \frac{T}{E^*}$. A critical interaction exists, beyond which magnetization formation occurs. The critical interaction increases as the temperature increases.

TABLE I. Bulk gap vs $U_c = \frac{g_c n_e}{8}$ for $n_e = 5 \times 10^{13}$ cm^{-2}.

	v_0 (eV nm)	λ (eV nm^3)	Δ_{bulk}(eV)	U_c (eV)
Bi_2Te_3	0.255	0.25	0.16	0.35
Bi_2Se_3	0.355	0.128	0.078	0.066

electron density on the surface. We will use ARPES data of Bi_2Te_3 and Bi_2Se_3 surfaces[9,13] to compare the critical interaction energy with the bulk energy gap for a typical surface density (Table I). In both materials $U_c < \Delta_{\text{bulk}}$, which puts the mean-field results within the necessary condition for the validity of the approximation.

At nonzero temperatures the transition happens when the free energy of the magnetized surface is lower than that of the nonmagnetized one.

It is useful to note that $\langle\sigma_{z-}\rangle = -\langle\sigma_{z+}\rangle \equiv \langle\sigma_z\rangle$. For $\mu = 0$, the equation for m becomes

$$m = \int \frac{d\boldsymbol{k}}{(2\pi)^2} \frac{x(m,\mathbf{k}) \tanh \frac{\sqrt{v_0^2k^2+x_m^2}}{2T}}{\sqrt{v_0^2k^2 + x_m^2}}, \tag{12}$$

where T is the temperature and $x(m,\mathbf{k}) = gm - \lambda k^3 \cos 3\theta$. The free energy difference (Δf) per unit volume is

$$T \int \frac{d\boldsymbol{k}}{(2\pi)^2} \log \left(\frac{1 + \cosh\left(\sqrt{v_0^2k^2 + x_m^2}/T\right)}{1 + \cosh\left[\sqrt{v_0^2k^2 + (\lambda k^3 \cos 3\theta)^2}/T\right]} \right). \tag{13}$$

It is natural to define the dimensionless temperature scale $\tau \equiv \frac{T}{E^*}$ where $E^* = (\frac{v_0^3}{\lambda})^{1/2}$ is the characteristic energy scale introduced by hexagonal warping. The resulting phase diagram is presented in Fig. 1.

As expected, the critical interaction strength g_c increases with increasing temperature. We note, however, that the effect on g_c is rather mild. Again, the phase transition is of second order, both for a fixed temperature as a function of g and for a fixed g as a function of temperature.

A similar analysis may be carried out to examine the conditions for in-plane magnetization to be formed. To that end, we assume a magnetization in the x-y plane, solve the self-consistent equation that determines its magnitude and find the conditions under which it leads to an energy gain. As we now show, for typical parameters (v_0,λ,k_Λ), the critical interaction strength to have in-plane magnetization $g_{c,x-y}$ is smaller than $g_{c,z}$, the critical interaction strength to have a magnetization perpendicular to the plane. However, as we also show, these parameters correspond to an extremely large warping parameter. Hence, the interesting quantity is the out-of-plane magnetization. We carry out the calculation at zero temperature. We note that an in-plane magnetization does not create a gap in the spectrum. It does, however, break time-reversal symmetry and hence removes the topological protection of the Dirac point.

The Bloch Hamiltonian is

$$\mathcal{H}(\boldsymbol{k}) = v_0(k_x\sigma_y - k_y\sigma_x) + \lambda k^3 \cos 3\theta \sigma_z - g\vec{m}\cdot\vec{\sigma}. \tag{14}$$

We denote $(m_x,m_y) \equiv \boldsymbol{m}_\parallel$. In the symmetry-broken phase, the system will choose a specific direction. Although the system is not rotationally invariant we find that the angle dependence is very small, and we choose $\boldsymbol{m}_\parallel = m_x$. The self-consistent equation for m_x is then given by

$$m_x = \int_{k_F}^{k_\Lambda} \frac{d\boldsymbol{k}}{(2\pi)^2} \langle\sigma_x(\boldsymbol{k})\rangle, \tag{15}$$

where

$$\langle\sigma_x\rangle = \frac{m_x g + v_0 k \sin\theta}{\sqrt{v_0^2k^2 + (gm_x)^2 + 2g v_0 m_x k \sin\theta + (\lambda k^3 \cos 3\theta)^2}}.$$

All that is left now is to solve Eq. (15), minimize the energy, and deduce the critical interaction $g_{c,x-y}$. The resulting $g_{c,x-y}$ has the same form as Eq. (8), with $Y(p_\Lambda)$ being replaced by $\Psi(p_\Lambda)$, where $\Psi(p_\Lambda)$ is a continuous, positive, and monotonically increasing function of p_Λ with the following asymptotic behavior:

$$\Psi(p_\Lambda) \sim \begin{cases} \frac{p_\Lambda}{4\pi}, & p_\Lambda \ll 1 \\ 0.352, & p_\Lambda \gg 1, \end{cases} \tag{16}$$

The ratio $\frac{g_{c,x-y}}{g_{c,z}} = \frac{Y(p_\Lambda)}{\Psi(p_\Lambda)}$ is presented in Fig. 2 for $\mu = 0$. For $k_\Lambda < 3.7\sqrt{\frac{v_0}{\lambda}}$, the instability to m_z appears before the instability to in-plane magnetization. Since this value of k_Λ corresponds to a warping parameter that is about a hundred times larger than that observed in Bi_2Te_3, we conclude that the interesting quantity to examine is the magnetization in the z direction. This conclusion does not change when the chemical potential is away from the Dirac point. We also considered the possibility of a tilted magnetic order. Expansion of the self-consistent equations reveals that near the phase transition line the magnetization is solely out-of-plane or in-plane.

Our analysis has so far been focused on the contact interaction between electrons, and has uncovered an instability of the surface to the formation of magnetization, with the instability being strongest for the formation of out-of-plane magnetization at zero temperature and zero chemical potential. The dependence of the critical interaction strength on temperature and chemical potential is however rather weak.

Motivated by these observations we turn to the long-range Coulomb interaction, $V(\boldsymbol{R}) = e^2/R$, and study the instability to the formation of out-of-plane magnetization at zero temperature and zero chemical potential.[14] We assume that

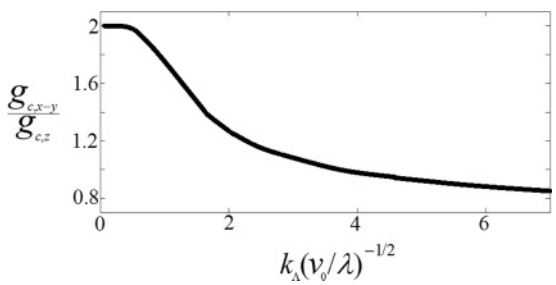

FIG. 2. Ratio between the critical interactions to have in-plane/out-of-plane magnetization as a function of the ratio of k_Λ to the warping wave vector scale $(v_0/\lambda)^{1/2}$. For typical values the instability to m_z occurs before the one to m_x.

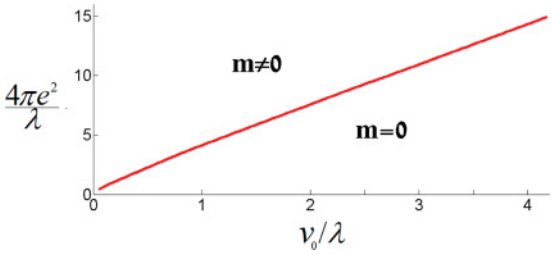

FIG. 3. (Color online) Phase diagram for Coulomb interaction at zero temperature. A critical interaction exists, beyond which magnetization formation occurs.

$\langle \psi^\dagger_\sigma(\boldsymbol{r})\psi_{\sigma'}(\boldsymbol{r}')\rangle \equiv M(\boldsymbol{R})\sigma_z$ is an exponentially decaying function of R with a decaying length α^{-1}. This assumption yields two self-consistent equations for the magnetization and for α:

$$m = \int \frac{d\boldsymbol{k}}{(2\pi)^2} \frac{\frac{4\pi me^2}{\sqrt{k^2+\alpha^2}} - \lambda k^3 \cos 3\theta}{\sqrt{v_0^2 k^2 + \left(\frac{4\pi me^2}{\sqrt{k^2+\alpha^2}} - \lambda k^3 \cos 3\theta\right)^2}}, \quad (17)$$

$$\frac{m}{\alpha} = \int \frac{d\boldsymbol{k}}{(2\pi)^2} \frac{\frac{2\pi me^2}{k\sqrt{k^2+\alpha^2}} - \lambda k^2 \cos 3\theta}{\sqrt{v_0^2 k^2 + \left(\frac{2\pi me^2}{\sqrt{k^2+\alpha^2}} - \lambda k^3 \cos 3\theta\right)^2}}. \quad (18)$$

The trivial solution, in which $m = 0$ and α is arbitrary, is always an exact solution to the equations above. After solving numerically for m and α and minimizing the energy, we identify the regions of parameter space in which a nontrivial solution exists, as shown in Fig. 3. The values we obtain for α^{-1} range between 1 and 4 lattice constants, hence justifying the interpretation of m as the magnetization.

For the Coulomb interaction the mean interaction energy per particle is of the order of $e^2 r_0^{-1}$, where r_0 is the mean distance between electrons on the surface. We can estimate $r_0 \sim n_e^{-1/2}$.

For a given density we can parametrize the critical interaction strength by defining a critical interaction energy $U_c = e_c^2 r_0^{-1} \sim e_c^2 n_e^{1/2}$. Again, for our approximation to be valid we must have $U_c < \Delta_{\text{bulk}}$.

We find this condition to be satisfied for both Bi_2Te_3 and Bi_2Se_3: Using Fig. 3 and extracting the density from ARPES data we evaluated the critical interaction strength, $e_c^2 \sim 0.057 e_0^2$ ($0.072 e_0^2$) for Bi_2Te_3 (Bi_2Se_3), where e_0 is the electron charge in vacuum. We find the actual Coulomb interaction on the surfaces of these two materials to be too weak for an instability. The dielectric constant on the two surfaces is close to 40, as compared to a value of about 15 for which our approximation leads to an instability.

To summarize, we examined here the possibility that time-reversal symmetry is spontaneously broken on the surface of a three-dimensional strong topological insulator due to interactions between surface electrons. We assumed that the surface can be described by a two-dimensional effective Dirac Hamiltonian, and we treated interactions within the Hartree-Fock approximation. We found that for a strong enough interaction, both of the contact and the Coulomb types, the surface is unstable with respect to the formation of spontaneous magnetization, with the strongest instability being the formation of magnetization in the direction perpendicular to the surface. For the contact interaction, we found the transition from the nonmagnetized to the magnetized surface to be of second order, both at zero temperature as a function of interaction strength and for a fixed interaction strength as a function of temperature. The dependence of the critical interaction strength on temperature and chemical potential, at least for the contact interaction, is rather mild. We found the interaction strength in the two most studied strong topological insulators to be too weak for an instability, but not by a large factor, making the instability an issue that may be relevant for other topological insulators. In particular, in order to see the phase transition one should seek a material with a large bulk energy gap, small velocity of the surface mode, and low dielectric constant.

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