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A Chemical Theory of Topological Insulators

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Research on topological insulators (TIs) has experienced an exponential growth in the last years, promising new technological applications in fields ranging from electronics to quantum computing. However, the strong condensed matter physical background that is needed to understand the exotic electronic structure of TIs has precluded its dissemination into the chemistry community. In this work we use chemistry-like models (e.g. the Hückel model) to bridge this gap. By taking bond alternating polyacetylenes as a starting point, we show how several key concepts about TIs, such as chiral symmetries or topologically-protected edge states, may be rephrased in terms of traditional chemical concepts by using Lewis resonance structures and bonding descriptors that characterize electron delocalization in real space. Overall, this Highlight should provide the background for understanding the properties of topological insulators to a broad chemistry readership.

1 Introduction

The last decade, the field of condensed matter physics experienced a revolution with the prediction^{1–3} and experimental realization^{4,5} of the so-called topological insulators (TIs)^{6,7}. This new quantum state of matter instantly became a hot topic in other areas of physics and materials science^{8–10}. In the chemistry community, however, topological insulators have not had the same widespread reception. While there have been several articles published in chemistry journals, their content has been mostly related to the physical or material science aspects of these systems. The aim of these articles has been to introduce TIs to chemists by presenting their phenomenology, exotic electronic structure, realiza-

tions in real-world materials and potential applications, but they have avoided delving into their theoretical characterization^{11–13}. Recently, Bradlyn *et al.*¹⁴ have developed a theory of “topological quantum chemistry”, which covers the full spectrum of topological materials, but which requires a strong physical background. Furthermore, this theory does not describe the chemistry behind these compounds.

One of the causes for this gap is the difference in the language and the methods of reasoning used by condensed matter physicists and theoretical chemists. In this article, we aim to scrutinize the simplest TI model, in order to provide thorough and detailed explanation of its theory from the point of view of a chemist, which would result in bridging the aforementioned gap.

TIs are insulators in the bulk, but with conducting states present on their surface. These surface states are pretty peculiar; they are *topologically protected*, in the sense that they remain conductive for as long as certain symmetries are preserved (we elaborate on the exact meaning of this statement in the next section). Moreover, the “protection” is independent of the surface cleanliness, disorder, passivation, etc. Under all these conditions, the surface (or interface) states will remain conducting.

These unique features make TIs the subject of intense research for their application in low-power electronics¹⁵, molecular-based spintronics¹⁶, next-generation solar cells¹⁷, quantum computing¹⁸, photonics¹⁹, novel organometallics²⁰, etc. Interestingly, the conducting surface states of TIs have attracted attention in catalysis²¹ and also playing the role of an electron reservoir that enhances the catalytic properties of noble metals supported on TIs^{22–24} or even for crystallization²⁵.

The most famous TIs belong to the Bi₂Se₃ family, which displays a single Dirac cone (*i.e.* electrons behaving like relativistic massless fermions) centred at Γ , the origin of the Brillouin zone. We call this particular kind of TIs \mathcal{L}_2 , and it can be shown that they need time-reversal symmetry in order to be preserved (*e.g.* no magnetic fields or impurities are allowed).

The theory related to the \mathcal{L}_2 subset of TIs is involved. However, simpler models more appealing to chemists do exist, which enable

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the understanding of the TIs' properties on chemical grounds. In this paper, we review the famous Su-Schrieffer-Heeger (SSH) model of polyacetylenes, providing some insight into their chemistry from standard chemical models and bonding descriptors.

2 Theoretical framework: The Hückel-like Model of Polyacetylene

Polyacetylene is the simplest conjugated polymer, with chemical formula $(\text{CH})_{2N}$. It is formed by alternating blocks of -CH- groups coupled by single and double bonds. Su, Schrieffer and Heeger (SSH) provided a very simple characterization of polyacetylenes by means of a tight-binding model²⁶. An excellent introduction to the topological features of this model is given by Ásboth *et al.*²⁷ Here, we adapt it to a Hückel formulation as well as to widespread chemical concepts.

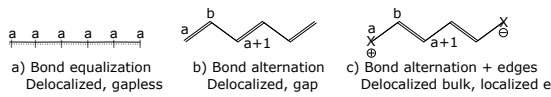


Fig. 1 Chemical representation of the resonance forms of interest in 1,3,5-hexatriene

Within the Hückel formalism, conjugated systems are usually treated by ignoring hydrogen atoms and considering only a single orbital, ϕ_i , -and a single electron- per carbon atom. Conjugation is introduced by means of a set of alternating single and double bonds, and only nearest-neighbour interactions are considered. Under these approximations, the effective one-electron Hamiltonian matrix elements are α , the on-site energy and β , the nearest-neighbour interaction:

$$\alpha = -\langle \phi_i | H | \phi_i \rangle \quad (1)$$

$$\beta = -\langle \phi_i | H | \phi_{i+1} \rangle \quad (2)$$

This minimal model provides a rather good description of aromatic molecules (e.g. benzene), where the resonance between different Lewis structures leads to bond equalization (see Fig. 1a). This is not the case in conjugated linear molecules, such as polyacetylene, where bond alternation is observed. To overcome this deficiency, it is possible to introduce two different nearest-neighbour interactions, β and β' (see Fig. 1b) :

$$\beta = -\langle \phi_{i,a} | H | \phi_{i,b} \rangle, \beta' = -\langle \phi_{i,b} | H | \phi_{i+1,a} \rangle, \quad (3)$$

The subscripts a, b refer to the new symmetry of the system. Indeed, upon bond alternation, the unit cell of the polymer is doubled. Under this scenario, we can observe two inequivalent carbon positions: those having the double bond to their right, and those having it to their left. Hence, in the i -th unit cell there are two carbon atoms, labelled a_i and b_i , that contribute to the bond-alternated Hückel Hamiltonian with $\phi_{i,a}$ and $\phi_{i,b}$ orbitals (see Fig. 1b). Assuming the same notation as in Fig. 1b, we intend β , the interaction between a_i and b_i , to represent the double bond interaction, whereas β' in between b_i and a_{i+1} is intended to represent the single bond (i.e. $\beta > \beta'$).

In what follows, we will ignore the on-site energy ($\alpha = 0$), which is valid as long as it has the same value for each atom (i.e. all atoms are equivalent). With this in mind, the Hückel-like Hamiltonian of polyacetylene can be written as

$$H = - \begin{pmatrix} 0 & \beta & 0 & 0 \dots \\ \beta & 0 & \beta' & 0 \dots \\ 0 & \beta' & 0 & \beta \dots \\ 0 & 0 & \beta & 0 \dots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \quad (4)$$

A direct diagonalization of H without using periodic boundary conditions gives two qualitatively different outcomes (see S.I. for a more detailed mathematical development), in the chemistry jargon: to two different resonance forms.

The first one is known within the physics community as the normal or *trivial* case, $\beta > \beta'$; it corresponds to the resonance form with the biggest weight since it has no charges (Fig. 1b). In this regime, there is a clear energy gap between the highest occupied (HOMO) and the lowest unoccupied (LUMO) molecular orbitals (Fig. 2a left). In the case of infinite systems this bandgap is given by $2(\beta - \beta')$. Orbitals display the usual delocalized behavior we would expect for a conjugated π system (Fig. 2a right).

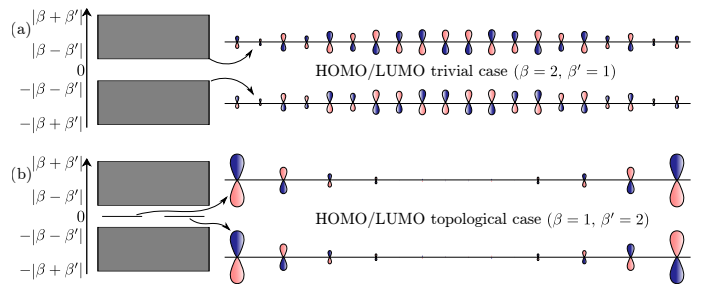


Fig. 2 Energy bands (left) and HOMO/LUMO coefficients (right) for the SSH solutions of $(\text{CH})_{20}$. (a) trivial solution ($\beta > \beta'$) (b) topological solution ($\beta < \beta'$)

As $\beta \rightarrow \beta'$ and the distinction between single and double bonds vanishes (i.e., $\beta = \beta'$), the model falls back into the common Hückel approach with bond equalization (Fig. 1a). For very large chains, this means that the system becomes (virtually) gapless (metallic) (see S.I. for the band gap and frontier molecular orbitals). Note that just as in other monodeterminantal models, Mott insulator solutions are not possible within this model.

Now we can assume, just like with benzene, that conjugated double bonds can easily lead to resonance and study the structure represented in Fig. 1c. This is equivalent to saying that $\beta' > \beta$ and mathematically, it constitutes a second family of solutions.

But why is this a qualitatively different family? The resonance form where $\beta' > \beta$ has two edges (Fig. 1c). Two new energy levels appear on top of the previous energy distribution, located in the middle of the band gap (that is at zero-energy, see Fig. 2b-left); these become the new HOMO and LUMO orbitals of the system, which are non-bonding. Since they do not mix with the rest of the chain, they remain very localized. Fig. 2b-right shows the corresponding orbitals. It can be seen that, unlike the orbitals in

the rest of the chain, the two new ones do not delocalize over the bulk, but remain rather localized on the edges. Moreover, since they are formed from just two edges, a bonding and anti-bonding pair is formed (the phase opposition can be seen toward the right border). Note that the overlap between the atomic orbitals (located on opposite edges) that contribute to these two molecular orbitals is very small, which explains why they virtually have the same energy. These states are rather special: their existence is independent of the actual value of β and β' (as long as $\beta' > \beta$). This fact explains the so-called “protection” of topological insulator properties upon changes in β and β' , i.e. upon changes in the interaction strengths. The second solution of the SSH model can be understood as the simplest case of *topologically protected edge states*.

In the remainder of the paper we elaborate on the chemical conditions to set up a topological insulator within this simple well-known model and the properties that can be derived from it which are relevant to chemists.

3 Chemical analysis of chiral symmetry

Why does this model of polyacetylenes show protected zero-energy edge states? The answer resides in its bipartite lattice, i.e. in bond alternation of equivalent atoms. This leads to an extra symmetry, known as *chiral symmetry*. Please note that the “chirality” concept is used as in condensed matter physics. In condensed matter physics, a Hamiltonian H has a symmetry represented by a unitary operator U if $UHU^\dagger = H$. We say that a system has a chiral symmetry if there is a unitary operator Γ such that $\Gamma H \Gamma^\dagger = -H$. Please note that this is not the common use of the “chiral” word in chemistry.

3.1 Conditions for chiral symmetry

3.1.1 The lattice is formed by two sub-lattices

Let us return to the Hamiltonian matrix H (Eq. 4). Since the labelling of the atomic orbitals is irrelevant (i.e. the Hamiltonian operator is symmetric under the permutation of the electrons), the H matrix can be written into an explicit block-diagonal form (see S.I.). This leads to the sublattices a and b behaving like “independent” lattices from each other. If a charge is situated on a given center b_i , resonance forms will only delocalize the charges along the b_i ($i = 1, N$) centres (Fig. 3a). Of course the same applies to the a sub-lattice. This result is well known within aromatic compounds in chemistry (Fig. 3b). A charge located on a benzene ring in the ortho position (b_1 in Fig. 3b) will be delocalized over other para (position b_2) and ortho (b_3) positions, but not over the meta (a_2, a_3) positions.

It is clear that transforming the trivial phase ($\beta > \beta'$) into the topological one ($\beta < \beta'$) or viceversa in a continuous way (i.e. adiabatically) implies closing the gap ($\beta' = \beta$). This implies crossing through a situation with fully equalized bonds, which in the limit $\beta \rightarrow 0$, means passing through an atomic situation (see S.I. for a more in-depth explanation).

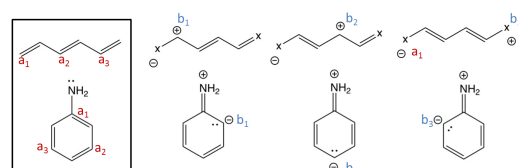


Fig. 3 a) Delocalization of charges in the bulk of one sub-lattice for hexatriene b) Delocalization of charges in aniline

3.1.2 Energies come in pairs

Chirality also implies important consequences on the MO diagram of the system. If ψ is a solution of the one-electron Schrödinger equation, $H\psi = E\psi$, there must be another solution with opposite eigenvalue, $-E$ (see S.I. for more details). Therefore all states must come in pairs with energy values $\{E, -E\}$. These are called *chiral partners*.

This property is also preserved in the $\beta = \beta'$ limiting case (i.e. normal Hückel). Let us examine the well-known solution of butadiene (the simplest 2N conjugate hydrocarbon) at $\alpha = 0$. The energies and molecular orbitals of the four one-electron states are given by:

$$E_1 = +1.6\beta, \quad \pi_1 = 0.37\phi_1 + 0.6\phi_2 + 0.6\phi_3 + 0.37\phi_4 \quad (5)$$

$$E_2 = +0.6\beta, \quad \pi_2 = 0.6\phi_1 + 0.37\phi_2 - 0.37\phi_3 - 0.6\phi_4 \quad (6)$$

$$E_3 = -0.6\beta, \quad \pi_3 = 0.6\phi_1 - 0.37\phi_2 - 0.37\phi_3 + 0.6\phi_4 \quad (7)$$

$$E_4 = -1.6\beta, \quad \pi_4 = 0.37\phi_1 - 0.6\phi_2 + 0.6\phi_3 - 0.37\phi_4 \quad (8)$$

It can be observed how $E_1 = -E_4$ and $E_2 = -E_3$, correspond to the two chiral pairs. They are related by a change of sign on the b sublattice (ϕ_2, ϕ_4), which transforms the chiral pairs: π_1 into π_4 , and π_2 into π_3 . This general rule for constructing energies and molecular orbitals within the Hückel approach is a direct consequence of the chiral symmetry of the even number of carbons chain.

As we saw before, these MOs are delocalized over the whole system and have support (non-zero coefficients) on both sub-lattices. This is apparent in the butadiene example as well as in bigger polyacetylenes. Fig. 2a shows how the MOs are delocalized over the whole unit, with both the HOMO and the LUMO displaying contributions in both sub-lattices. However, this is not the case at the borders. When a state has zero-energy, $E = -E = 0$, the chiral partners become degenerate and they can be chosen to have support on only one of the sub-lattices, either a or b . This is easily seen in the leftmost structure of Fig. 3a. Due to the pairing, one edge belongs to the a sub-lattice and the other edge belongs to the b sub-lattice. Hence, the state on the left (right) has non-vanishing contributions only in the a_i (b_i) sites.

Graphene is a system similar to polyacetylene in 2D. Its honeycomb lattice is bipartite (two C atoms in each cell), making it a “chiral” material. Unlike polyacetylene, all the bonds in graphene have the same strength ($\beta = \beta'$), making it a very special conduc-

tor.

3.2 Lifting the conditions

In order to obtain the peculiar properties of a topological phase, chirality needs to be set up: an even number of centres with zero on-site energy. When one of these requirements is switched off, chirality is lost. We illustrate the consequences of this set-up with two simple examples.

3.2.1 The bipartite lattice

If we take a system with an odd-number of conjugated carbons, the $(E, -E)$ correspondence breaks down. For example, the Hückel model for the allyl cation (3 centres) under bond equalization conditions and $\alpha = 0$, would lead to

$$E_1 = -\sqrt{2}\beta, \quad \pi_1 = \phi_1 + \sqrt{2}\phi_2 + \phi_3 \quad (9)$$

$$E_2 = 0, \quad \pi_2 = -\phi_1 + \phi_3 \quad (10)$$

$$E_3 = \sqrt{2}\beta, \quad \pi_3 = \phi_1 - \sqrt{2}\phi_2 + \phi_3 \quad (11)$$

Molecular orbitals π_1 and π_3 are connected by a change of sign in the a and b sub-lattices. One non-bonding orbital does appear (π_2), but it is not protected, since it has no partner imposed by symmetry.

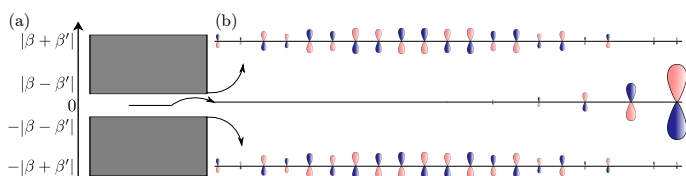


Fig. 4 Chain with 21 atoms, $\beta = 2$ and $\beta' = 1$. (a) Energy diagram. (b) Orbitals close to the Fermi level. Reversing β, β' just localizes the zero-energy level to the left side.

Fig. 4 shows the results for the energy and the frontier molecular orbitals for $N=21$ ($\beta \neq \beta'$). Since we have an odd number of π electrons, the highest occupied molecular orbital is singly occupied (SOMO for Singly Occupied Molecular Orbital). The non-bonding state is localized just on one end.

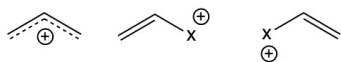


Fig. 5 Resonance scheme for allyl cation

This can be understood if we analyze the resonance forms of the allyl cation. Since the number of carbon atoms is odd, only one border appears. The resonance form in Fig. 5-center is the solution for $\beta > \beta'$ whereas the resonance form in Fig. 5-right corresponds to $\beta' > \beta$. It can be seen that, contrary to what we had found for a bipartite network, these two solutions are the same. Hence, the absence of a bipartite lattice destroys the existence of two different solutions or “phases”.

As a side note, the $\beta = \beta'$ solution in Eq. 11 (Fig. 5a) corresponds to a delocalized SOMO along with a complete delocaliza-

tion of the charge. For a large number of atoms this would lead to a metallic system just like that of the bipartite case.

3.2.2 The on-site energy

The chirality is also broken upon distortion of the same on-site energy. If we change the on-site energy of the atoms in one of the sub-lattices (*i.e.* by adding a difference of potential ΔV between atoms in positions a_i and b_i), the Hamiltonian is no longer split in two blocks (see S.I. for more details). From the chemical point of view, this is equivalent to considering a network of different atoms, type A atoms on sites a_i and type B ones on sites b_i ; for example, a $(-C-N-)_n$ chain instead of polyacetylene (Fig. 6b). The potential, ΔV , means that different atoms have different on-site energies, *i.e.* they have different values of electronegativity. Fig. 6 illustrates this way of breaking chirality. While C_3N_2 preserves the odd number of atoms and has a two-center unit-cell, the Hamiltonian cannot be written in a block-diagonal form. The different probability of holding charges on the different atoms, C and N, gives rise to additional possibilities of delocalization so that charges delocalize over the full chain, both on a and b centres (Fig. 6a and 6c).

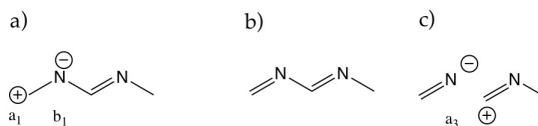


Fig. 6 Delocalization of charges when $\alpha_a \neq \alpha_b$ (*i.e.* $\Delta V \neq 0$).

3.3 Topological phase transitions

Why is the $\beta' > \beta$ set of solutions called topological? Topology is the branch of mathematics concerned with the study of space and its continuous transformations. For instance, an orange is a body with no holes. We can easily imagine a continuous transformation from an orange shape to a dish shape (just by smashing a sphere of Play-Doh[®]). This means they are topologically equivalent, an equivalency that is identified by the fact that none of them has holes. A donut has as many holes as a pottery mug. Hence, they are topologically equivalent. Putting this together, the donut and the orange belong to different topological classes. This equivalency is represented by a number, the number of holes or *genus*. The fact that a different number of holes is allowed, enables the existence of “topological phases”.

The existence of chirality in the SSH model ensures the possibility of the onset of a topology in the electronic structure, *i.e.* the possibility of having two phases which can be connected in a continuous manner (*i.e.* changing the single-double bond lengths) and with very different physical properties. Within this topology, the hexatriene in Fig. 1a is equivalent to all phases where $\beta > \beta'$. For example, it is equivalent to 3 double bonded dimers ($\beta' = 0$). This is similar as to transforming the orange into a disk.

The other topological phase of the model has $\beta < \beta'$. Taking the resonance form from Fig. 1c, if we now stretch the single bonds (decrease β), we end up with two double bonded dimers and two borders, which corresponds to a different topological phase, like

the donut in the analogy. The link between both phases occurs for all the $\beta = \beta'$ cases.

What plays the role of genus in the electronic structure? Topological phases are usually characterized by the so-called “winding number”, γ . In our case (see S.I. for more details), γ is 0 for the trivial case ($\beta > \beta'$) and 1 for the topological case ($\beta < \beta'$). The marginal case $\beta = \beta'$ does not have a well-defined winding number*.

What are the consequences having topological phases? Since there are only two ways of undefining γ , each phase is said to be “topologically protected”. β and β' can be changed at will as long as we remain within the same topological region. There are just two ways of undefining γ . The first option is to have zero-energy states, which means changing from one topological phase to another crossing through $\beta = \beta'$ and hence passing through a metallic state. The other option is to break the chiral symmetry. This would mean including a term on its diagonal like in Section 3.2.2, when different atoms were introduced.

It should be noted that the edge states must not necessarily be located on the extremes of the chain, which leads to different domains in the polyacetylene molecule (see Fig. 7 and S.I. for more details).

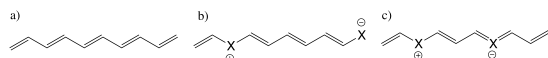


Fig. 7 Resonance structures leading to domain walls: (a) regular bipartite lattice, (b) lattice with one domain wall and one non-bonding atom and (c) lattice with two domain walls. Each domain wall separates a region with “topological” order from one with “trivial” order.

Why are the topologically protected edges states so robust? The interaction parameters (β , β') can be changed at will, but the winding number in the chains has to remain $\gamma = 1$ if the phase is left unchanged. In this manner, we could retain the two different resonance forms at very different pressures (changing the absolute values of β and β'). However, if we break the chiral symmetry (e.g. with impurities that introduce a V term in the Hamiltonian), the topological properties are lost.

4 From the model to real systems

We now convey how the SSH model we have chemically developed can assist in understanding the properties of real topological insulators. TIs are insulator materials in the bulk, but with conducting states at their surfaces. However, these surface states have very peculiar properties: they are topologically protected,

in the sense that they remain conducting as long as the protecting symmetry is preserved (for example, the chiral symmetry we have seen). The surface (or interface) states remain conductive independently of the surface cleanliness, disorder, passivation, etc. Moreover, scattering and dissipation are heavily suppressed in these states.

4.1 Two-dimensional SSH-model

Extending the concepts developed here with the SSH model to two- or three-dimensions is straightforward (but lengthy). However, we can use hand-waiving arguments to understand the general behaviour of TIs. Let us assume we make an equidistant array of SSH hydrocarbons and place them at a medium interaction distance. If each SSH-like strand is in the trivial phase, no edge state is to be expected, and the result is a trivial 2D insulator. Instead, if the chains are in the topological phase, the 2D object will have two regions:

- The bulk of the hydrocarbon chains. Since chains are far apart, neighbouring chains will only lead to weak interactions that slightly perturb the local electronic structure. This can be viewed just like a stacking of polyacetylene molecules, where the π stacking dominates, but the general molecular orbital scheme is unaltered. Hence, they remain insulating. This part will be just the same as the bulk in the SSH model (localized, with bond alternation, localizable orbitals)
- The borders. These are isolated “atoms”, all placed at the same distance. If β_2 represents the interaction related to this new dimension, it results that all the border atoms interact with the same β_2 value. This indicates that a delocalized interaction (metallic state) is settled in between the edges.

Hence, we retrieve TIs protected characteristics: insulating bulk and conducting surface, which must remain metallic –unless the chiral symmetry is broken.

Although these arguments are hand-waiving, they are meant to give an idea of the general features of topologically protected states, which can be transposed to real-world examples such as graphene²⁸ and black-phosphorus nanoribbons.²⁹

Unfortunately, the above holds only as long as the chiral symmetry is not broken. But we have seen that an atom with different electronegativity leads to the breaking of the chiral symmetry. Therefore, chemisorption of foreign atoms in these models ends with the TI state, which is not the case for the most commonly used TIs. This happens because these systems set up their topology with a symmetry that is resilient to doping.

4.2 Topological insulators with time-reversal symmetry

To find a more robust symmetry, we restate the sub-lattice symmetry of a conjugated polymer. Instead of using the chiral symmetry, given by “*there are two identical but inequivalent atoms per unit cell*”, we make the following slight change to the statement: “*there are two identical but inequivalent spins per unit cell*”. After replacing the sub-lattices a, b with the spins *up, down* the analogy in the Hückel formulation is straight forward. To have the

* The name winding comes from Berry phases. The phase of a periodic system needs to be periodic, for instance $\phi(k=0) = \phi(k=2\pi) = \phi_0$. In a topologically trivial system, if we go to the molecular limit by weakening the weaker bond $\beta \rightarrow 0$, we will get $\phi(k) = \phi_0, \forall k$ (i.e. the reciprocal space becomes irrelevant). Conversely, in a non-trivial system, the wavefunction acquires an extra phase -Berry or Zak phase- but without breaking the periodicity of the wavefunction, this can be achieved if $\phi(k=0) = \phi_0$ and $\phi(k=2\pi) = 2\pi + \phi_0$. If we try to reach the molecular limit by letting $\beta' \rightarrow 0$ we will fail, the extra phase 2π “winding” around the reciprocal space prevents to reach the molecular limit. In simpler terms, the extra phase prevents the reciprocal space from becoming irrelevant, and in the SSH model this is due to the stronger bond is between adjacent unit cells

chiral symmetry in the SSH model both sub-lattices must be identical (i.e. the same electronegativity). The new spin-based symmetry is rather translated into: the total bulk spin must be zero (spin unpolarized) or, as physicists call it, the time-reversal symmetry has to be preserved. The use of spin -instead of the sub-lattice degree of freedom- is very convenient, since a magnetic field or magnetic impurity is needed to break the time-reversal symmetry. Otherwise, the topological features will hold. In other words, non-magnetic impurities will not destroy the metallic surface states.^{30,31}

In some materials with heavy elements, such as Bi₂Se₃, Bi₂Te₃ and Sb₂Te₃, the spin-orbit coupling is large enough to change the nature of the wavefunction, mixing the valence and conduction band. This triggers the transition to a topological state. The surface states (“edges”) of these materials are spin polarized in reciprocal space; just like the SSH model topological phase had a net dipole (charges + and –) in the edges/interfaces. Hence, instead of having two split sub-lattices, now we have a spin-split system. Still, the net spin moment averages to zero (just like the charges did in the SSH model), preserving the time-reversal symmetry. This means that it is possible to set up the system such that different current senses have different spins, so that the “turning around” must also flip the spin. The result is that dissipation in these states ends up being heavily suppressed, making the proposed time-reversal TIs a promising venture for spin-based electronics³².

More specifically, these systems are especially useful in low-energy consumption electronics¹⁵, molecular-based spintronics¹⁶, next-generation solar cells¹⁷, quantum computing¹⁸, photonics¹⁹, novel organometallics²⁰, and many more. Most recently, the conducting surface states of TIs have also attracted attention because they could play the role of an electron reservoir that enhances the catalytic properties of TI-supported noble metals^{22–24,33,34}.

5 Conclusions

While the prediction and experimental realization of topological insulators constituted a revolution in material science, the language gap between physicists and chemists has precluded the expansion of the field the general chemical jargon. This Highlight shows that the main concepts involving topological insulators can be understood by introducing a slight variation of the familiar Hückel formulation.

We show that the existence of topological phases in a bond-alternating polyacetylene model is due to an extra symmetry, known as “chiral symmetry”. It sums up to two characteristics: the network is entirely made of the same atoms, and all the π electrons come from double bonds, so that the chain has $2N$ π electrons. The above two features ensure that everything comes in pairs: all atoms have a “partner” (through the double bonds), and so do eigenvalues (energies) and eigenvectors (molecular orbitals). This simple model enables us to understand the meaning of edge states, topological protection and other basic concepts in the theory on TIs -all in terms of standard chemical concepts such as Lewis resonance structures.

Although the model is simple, we have shown that the ap-

proach presented in this work enables chemists to understand the properties of real systems such as black phosphorous or graphene ribbons, and even to construct hand-waving arguments that would extend this model to higher dimensions and more resilient (e.g. time reversal) symmetries.

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Conflicts of interest

There are no conflicts to declare.

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