First principles study of topological phase in chains of 3d transition metals

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Recent experiments have shown the signatures of Majorana bound states at the ends of magnetic chains deposited on a superconducting substrate. Here, we employ first principles calculations to directly investigate the topological properties of 3d transition metal nanochains (i.e., Mn, Cr, Fe and Co) for isolated and surface–deposited wires. Our results stand in opposition to bulk calculations which have been previously used. From the obtained band structure, we found the exact tight binding model in the Wannier orbital basis with realistic parameters. For these models, we calculate topological invariant of $Z_2$ phase, from which we conclude that the non–trivial topological phase can exist only in Mn and Co (free–standing) chains. Additionally, we discuss non-collinear magnetic moments as a source of the non–trivial topological phase. We show that this type of magnetic order is not stable in the case of the Fe and Co wires and cannot be the source of the non–trivial topological phase in these systems. Finally, we discuss the influence of the substrate on the band structure and magnetic properties of the nanochain’s atoms. We show that the coupling of the chain to substrate leads to suppression of the magnetic moment value and to strong modification of the band structures.

I. INTRODUCTION

Prediction of localization of the Majorana bound states (MBS) at the ends of the one-dimensional chain [1] initiated intensive studies of this phenomenon in wide array of systems [2–5]. Typically, to generate MBS a mutual interplay between the conventional s-wave superconductivity, Zeeman magnetic field and strong spin-orbit coupling is essential [6, 7]. This condition can be achieved in semiconductor–superconductor nanostructures, where a semiconducting nanowire is deposited on a conventional superconductor [8–15]. Other theoretically predicted possibilities of the emergence of MBS, are chains of the magnetic atoms [16–19] or nanoparticles [20] located on a superconductor. The interplay between the magnetic moments and proximity induced superconductivity can drive the system into a topological phase [21, 22].

Scanning tunneling microscopy (STM) technique has been proven to be an excellent tool in this venue. The experiment based on the theoretical prediction was carried out in 2014 by Yazdani group [23] – the authors presented the evidence of forming of topological Majorana zero modes in iron chains on the superconducting Pb(110) surface. Additionally, high-resolution experiments with superconducting tips confirmed the existence of zero-energy excitations in this type of chain [24] and also, in the form of zero-energy local density of states (LDOS) measurement [25]. More recently, the spin-dependent experiments [26] demonstrated the emergence of the MBS in this system [27].

The mentioned experiments are based on the existence of the Yu–Shiba–Rusinov (YSR) in-gap bound states induced by a magnetic impurity [28–30]. The interaction of the local spin of impurity with the Cooper pairs in superconductor gives rise to a low-lying excited state within the gap of the quasiparticle excitation spectrum [31, 32]. Progress in experimental techniques allows the study of the YSR bound states of individual magnetic atoms [33]. Such studies of the YSR bound states were performed for many 3d transition metal adatoms, like e.g. Ti [34], Mn [33, 35–39], Cr [37, 38, 40, 41], Fe [42, 43], or Co [44]. Forming the chain of magnetic adatoms can lead to the evolution of the YSR bound states to the zero–energy MBS [45–47].

Experimentally, the monoatomic chains are usually prepared by the electron beam evaporation technique. This method was used successfully in the case of the

Figure 1. Schematic representation of a discussed system: the monoatomic magnetic chain of 3d transition metal (cyan atoms) at the surface of superconductor (gray atoms).
Fe [23–25, 27, 48] and Co [49] chains. However, recent progress in atomic engineering [50–54] allows for in situ construction of the magnetic atomic chains [55–62]. This technique can help to produce monoatomic chains on the superconducting surfaces (Fig. 1). In relation to chains prepared by electron beam technique [23–25, 27, 48, 49], artificial magnetic chains can have predetermined parameters, such as distance between atoms. Additional advantage of this technique is a possibility for preparation of ideally homogeneous system. By pushing this idea further, the pristine, homogeneous chains of 40 atoms and longer were produced [62] by Wiesendanger group, using an in-situ STM assembly [60]. The zero-energy MBS at the Fe chain ends became more stable with increase of the nanochain length.

In the context of the mentioned experiments, in this paper we study the physical properties of monoatomic chains of magnetic 3d transition metal atoms, i.e., Mn, Cr, Fe and Co. Our studies take advantage of first principles calculations and the parameters obtained using this method are applied in a tight binding model (TBM) in order to calculate topological invariants of the investigated systems. In the previous studies, the analysis of topological properties of monoatomic chains was based on tight-binding models with the hopping parameters taken from bulk crystals [23, 49]. Since the electronic band structures of monoatomic chains significantly differ from those of crystals, such simplified approach may lead to wrong conclusions. Surprisingly, our calculations for the 3d monoatomic chains show that a non-trivial topological phase may exist only in Mn and Co free-standing nanowires, while this phase is excluded in Fe or Cr chains. We study also the non-collinear magnetic order as a possible origin of topological phases as well as the impact of the substrate on electronic band structures of monoatomic chains. This paper is organized as follows. First, we describe in detail the methods of investigation (Sec. II). Next, we present and discuss our numerical results (Sec. III), and finally we summarize the results in Sec. IV.

II. METHODS

The ground state of electronic structure can be described by density functional theory (DFT) [63]. Typically, the electronic band structure is in a good agreement with experimental data given by e.g. angle-resolved photoemission spectroscopy (ARPES). In our study we adopted the following method of investigation: (i) DFT calculations of electronic properties and (ii) construction of a realistic TBM.

This corresponds to the comparison of the parameters obtained for bulk crystals with the results from calculations for isolated nanowires, i.e., an atomic chain in the absence of substrate. The parameters calculated for the atomic chains are used in the rest of our study. Finally, we find band structure for chains deposited on a superconducting substrate, which corresponds to realistic situation where the orbitals of atoms from the chain hybridize with the substrate orbitals (cf. Fig. 1).

A. Ab initio calculations

The DFT calculations were performed using the QUANTUM ESPRESSO code [64, 65]. The exchange-correlation functional was calculated within the generalized gradient approximation [66] developed by Perdew, Burke, and Ernzerhof [67]. The wave functions in the core region were evaluated using the full potential projector augmented-wave method [68, 69]. We performed calculations in the absence and in the presence of the spin-orbit coupling (SOC), using pseudopotentials developed in frame of PSLIBRARY [70]. Within the DFT calculations, we executed a full optimization of the structural parameters for conventional cells (for bcc and hcp structures) and primitive cells (for an isolated chain with vacuum layer of 10 Å).

Additionally, to study the impact of the additional neighbors in the chain states, we modeled a system with the substrate in approximated form, where the chain is coupled to one layer of superconducting substrate (containing three atoms of Pb) with vacuum layer of 10 Å. In calculations, we used the Monkhorst-Pack scheme [71] with 12×12×12 (12×12×4) k-grid in the case of Fe-bcc (Co-hcp) and 4×4×12 for isolated nanowires and nanowires deposited on Pb substrate. We have also used the cutoff for charge density with value suggested by using pseudopotentials increased by 100 Ry and cutoff for wave functions with value equal to quarter of the charge density cutoff.

B. Tight binding model

Using the band structure obtained from the DFT calculations, we can find the realistic TBM of the monoatomic chains in the basis of the maximally localized Wannier functions (MLWF) [72–74]. We perform this part of calculations using the WANNIER90 software [75, 76]. This allows for description of our system by using TBM in the form:

\[ \mathcal{H}_0 = \sum_{RR',\mu\nu,\sigma\sigma'} T_{\mu\nu}^{\sigma\sigma'}(R, R') c_{R\mu\sigma}^\dagger c_{R'\nu\sigma'}, \]

where \( c_{R\mu\sigma}^\dagger \) (\( c_{R\mu\sigma} \)) is the creation (annihilation) operator in the MLWF basis. Here \( T_{\mu\nu}^{\sigma\sigma'}(R, R') \) is the matrix describing the electron hopping from orbital \( \nu \) located at \( R' \) with spin \( \sigma' \) to orbital \( \mu \) located at \( R \) with spin \( \sigma \). In this description, the hopping without and with spin-flip component corresponds to the kinetic and spin-orbit coupling term, respectively.

When the chain is coupled to the superconductor, the superconducting gap \( \Delta \) can be induced by the proximity
effect. Then, our system can be described by the Hamiltonian:

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_{\text{SC}},$$  

(2)

where the first term denotes the “free” electrons (band structure), i.e., the Hamiltonian (1) in momentum space:

$$\mathcal{H}_0 = \sum_k H_{\mu \nu}^{\sigma \sigma'}(k) c_{k \mu \sigma}^\dagger c_{k' \nu \sigma'},$$  

(3)

where $H_{\mu \nu}^{\sigma \sigma'}(k) = \sum_{R, R'} \exp[i k \cdot (R - R')] T_{\mu \nu}^{\sigma \sigma'}(R, R')$. The second term, describes superconductivity and can be written in the BCS-like form:

$$\mathcal{H}_{\text{SC}} = \Delta \sum_{k \nu} (c_{-k \nu \uparrow} c_{k \nu \downarrow} + \text{h.c.}),$$  

(4)

where $\Delta$ is half of the superconducting gap (for lead $2\Delta \sim 2.7$ meV [37, 77–79]). Now, $c_{k \mu \sigma}^\dagger$ ($c_{k \mu \sigma}$) is the creation (annihilation) operator of the electron with spin $\sigma$ and momentum $k$ in orbital $\mu$.

C. Non–trivial topological phase

In the case of the one-dimensional hybrid semiconductor–superconductor nanowires [5, 8–15], the phase transition from a trivial to topological phase can occur, when splitting of the bands given by the spin–orbit coupling is larger than the superconducting gap [80–82],

$$\mu_B H_z = \sqrt{\tilde{\mu}^2 + \Delta^2},$$  

(5)

where $\mu_B$ is the Bohr magneton, $H_z$ is the magnetic field parallel to the nanowire, $\Delta$ is the superconducting gap, while $\tilde{\mu}$ is the Fermi energy computed at the bottom of the band. In our case, the magnetic moment plays the role of the effective “magnetic field”. Here, it should be noted, that in contrast to the hybrid nanostucture, realization of the topological phase is given only by the intrinsic properties of the monatomic chain, e.g. magnetic order or the position of Fermi level (which strongly depends on the type of atoms and the lattice parameters). Therefore, it is crucial to obtain the correct TBM of studied system and our proposed solution is to use the method described in the previous section.

The topological phase can be described by topological invariant, e.g. the winding number $w$ [83]. However, in our case, we describe the topological phase by the Pfaffian of the transformed Hamiltonian, which is a $\mathbb{Z}_2$ invariant [1]. This type of invariant can be defined for any system described by the Bogoliubov–de Gennes equations [84], which is equivalent to the Hamiltonian $\mathcal{H}$. Because our system has the particle–hole symmetry, i.e. $k = 0, \pi$ are the particle–hole symmetric points in the Brillouin zone [85], the Pfaffian is given by [84]:

$$Q = \text{sgn} \begin{vmatrix} \text{Det}(A(k = \pi)) \end{vmatrix} \text{Det}(A(k = 0)) = (-1)^w.$$  

(6)

Here, $A(k)$ denotes the element of Hamiltonian matrix in the block off-diagonal form [86], which can be derived from the unitary transformation $\mathcal{U}$ [87]:

$$\mathcal{U} \mathcal{H} \mathcal{U}^\dagger = \begin{pmatrix} 0 & A(k) \\ \bar{A}(k) & 0 \end{pmatrix},$$  

(7)

where $A_{\sigma \sigma'}^{\mu \nu}(k) = H_{\sigma \sigma'}^{\mu \nu}(k) + \Delta \delta_{\sigma \sigma'} \delta_{\mu \nu}$. The topological phase is realized when $Q = -1$.

III. NUMERICAL RESULTS

We start from a short description of the Fe bcc and Co hcp bulk systems. From the DFT self–consistent calculations, we find that the Fe bcc (Co hcp) structure have magnetic moments equal to $2.1988 \mu_B$ ($1.6693 \mu_B$) and lattice constant of $2.4512 \text{ Å}$ ($2.4881 \text{ Å}$). For the optimized systems, we find the electronic band structures (Fig. 2). In both cases, the 3d orbitals are accumulated around the Fermi level, while the rest of states (unoccupied 4p states) are located far above the Fermi level (approximately above 7.5 eV).

A. Isolated chains

Now we discuss the results for the isolated magnetic chains. Here, we performed the volume relaxation of one

![Image](attachment:image.png)

Figure 2. First Brillouin zone and band structures of the Fe bcc and Co hcp crystals. Results in the absence of the spin–orbit coupling. Red and blue colors denote the states with spin $\uparrow$ and $\downarrow$, respectively. Fermi level is located at zero energy.
Table I. Distances between atoms (in Å) and magnetic moments (in $\mu_B$) in the isolated chains.

| atom type | Cr  | Mn  | Fe  | Co  |
|-----------|-----|-----|-----|-----|
| distance  | 2.07| 2.30| 2.23| 2.15|
| mag. mom. w/o SOC | 1.77| 3.55| 2.94| 2.05|
| mag. mom. w/ SOC  | 1.78| 3.55| 2.95| 2.05|

magnetic atom with the 15 Å of vacuum in $\hat{x}$ and $\hat{y}$ directions (chain is aligned along the $\hat{z}$ direction). From this, we find the distances between atoms in the isolated nanowires (see Tab. I). The obtained distances in both Fe and Co chains are approximately 0.2 Å smaller than those in the bulk materials, while magnetic moments are larger. Modification of these two quantities must have a substantial impact on the parameters of the model describing the atomic chains. It is clearly visible in the band structures of the isolated chains (see Fig. 3). We observe a strong shift of the $p$-orbital states to lower energies (cf. Fig. 2 and Fig. 3, states initially located above 10 eV are shifted to energies around 4 eV). This leads to the strong hybridization between these states with the $3d$ levels. More importantly, one additional band crosses the Fermi level. In consequence, isolated monoatomic chains cannot be described not only by a simple single-orbital tight binding model, but even by a model incorporating as much as ten $3d$ orbitals.

The shapes of the obtained bands associated with $3d$ orbitals are approximately given as a cosine-like function of momentum (see Fig. 3), which is typical for a one-dimensional chain. However, when $3d$ states hybridize with other orbitals, a relatively large “deformation” of this shape (marked by green circle) takes place. Therefore, the band structure cannot be approximated by the dispersion relation of a simple one-dimensional lattice anymore. The other consequence is an avoided crossings behavior of the hybridized bands (marked by pink circle).

Introduction of the spin-orbit coupling in the calculations does not change the results qualitatively. As usually, the band degeneracy is lifted thanks to spin–orbit coupling, however, the shape of band dispersion is not influenced. The magnetic moments found in non-collinear calculations have approximately similar values, independently of its direction. Still, the largest splitting of the bands can be found when the magnetic moments are parallel to the nanowire. Even though splitting of the bands due to the spin-orbit coupling depends on the atomic mass \[88\], it is much smaller for isolated nanowires than in the bulk.

In conclusion, difference in distance between atoms in

Figure 3. Electron band structures of Cr, Mn, Fe, and Co nanowires (panels from a to d, respectively). Results obtained at absence of the spin-orbit coupling. Red and blue colors denote states with the spin $\uparrow$ and $\downarrow$, respectively. Fermi level is located at zero energy.

Figure 4. The same as in Fig. 3 in the presence of the weak spin-orbit coupling $\lambda \simeq 0.2$ eV and magnetic moment parallel to the nanowire. Solid pink lines and blue dots correspond to band structures obtained from the DFT and TBM calculations, respectively. Fermi level is located at zero energy.
chain and in bulk, as well as reduced number of neighboring atoms, leads to severe modification of most of system parameters e.g. hoping integrals, magnetic moments, or spin–orbit coupling. Additionally, $p$ type orbitals can also play an important role in the further description of the system.

**Realization of a non–trivial topological phase.** — In the previous studies of the magnetic monoatomic chains, the Slater-Koster tight-binding model parameters were used [23, 49], in order to describe nanowires capable of hosting the topologically non–trivial phase. In the case of the Fe chain, the hopping integral values were taken for the nearest-neighbor distance of the bulk Fe (bcc, $Im\bar{3}m$, Space group: 229), which is 2.383 Å [89]. Similarly, in the case of the Co chain, the hopping integral was calculated for the nearest neighbor distance of the bulk Co (hcp, $P6_3/mmc$, Space group: 194) with $a = 2.486$ Å [90]. Taking into account strong modifications of the band structure in the isolated chains (see Figs. 3 and 4), in particular a different number of bands crossing the Fermi level, such assumptions can lead to incorrect conclusions regarding the existence of the non–trivial topological phase.

To precisely describe the band structures of isolated chains, we found the TBM in the MLWF based on the DFT calculations (cf. Fig. 4). In a general case, the TBM model describing our system around the Fermi level is mostly composed of $d$-like orbitals (typical for transition metals). However, contrary to the bulk models, additional $p$-like orbitals should be included in the model.

Next, by employing these models, we calculate the topological number $Q$ given by Eq. (6). Additionally, we assume that the superconducting gap induced by the proximity effect in nanowires is equal 3 meV (which is close to the experimental result of 2.7 meV). That small, qualitative, difference does not change results, which are presented in Tab. II. As we mentioned before, the topological phase can be realized only when $Q = -1$. From our calculations we can conclude that the topological phase can be induced only in Mn and Co nanowires.

| $k$   | Cr | Mn | Fe | Co |
|-------|----|----|----|----|
| 0     | +  | +  | −  | +  |
| $\pi$ | +  | −  | −  | −  |
| $Q$   | +1 | −1 | +1 | −1 |

**B. Non-collinear magnetic moments**

A topologically non–trivial phase is not exclusive to a ferromagnetic chain – in some situations topological effects can also be induced by non-collinear magnetic moments. In the chain of one-orbital magnetic “atoms”, the spiral order can minimize the free energy of the system leading to the emergence of a topological phase [93, 94]. In this situation, the Majorana quasiparticles can be found at the end of the chain [21, 22, 46, 95]. This is possible due to the fact that the spiral magnetic order leads to the same effects as the spin-orbit coupling together with the external magnetic field [96, 97].

In a more realistic situation of a multi-orbital chain, the description using only a simple model may not be sufficient [17]. However, the DFT calculations allow for a comparison of the energies of the chains with different non-collinear magnetic orders (Tab. III). From this comparison, we can find the order which minimizes the energy of the system (values in the box). As we can see, in the case of Fe and Co atoms, the ferromagnetic order is more favorable. In Fe chain, the magnetic moment anteed. On the other hand, for the Co chain with the SOC number of crossings was even [49]. From our results (cf. Fig. 4), even number of band crossing the Fermi level within half of the Brillouin zone are realized in the Cr and Fe nanowire. These analyzes yield comparable results to those obtained from $Q$, supporting the hypothesis about realization of the non–trivial topological phase in Mn and Co nanowires.
Table III. Comparison of the energies between non-collinear magnetic orders with magnetic moments lying in the plane containing the chain \( (E_\parallel) \) and in the plane perpendicular to the chain \( (E_\perp) \), \( \delta E = E_\parallel - E_\perp \), which plays the role of the magnetic anisotropy energy. The angle of the magnetic moment rotation in space is given by \( \varphi \), which depends on number of the atoms in magnetic unit cell \( n \), i.e. \( \varphi = 2\pi/n \). All results in eV per atom come from calculation with the spin-orbit coupling present in the system.

\[
\begin{array}{cccccccc}
\varphi & \text{Cr} & \text{Mn} & \text{Fe} & \text{Co} \\
\hline
0 & -6.5 \times 10^{-4} & 4.2 \times 10^{-6} & -1.538 & -1.538 & -1.101 & -1.108 & -0.491 & -0.470 \\
\pi & -1.057 & -1.056 & -1.794 & -1.794 & -0.800 & -0.799 & -0.074 & -0.025 \\
2\pi/3 & -0.582 & -0.582 & -1.828 & -1.828 & -0.923 & -0.923 & -0.144 & -0.149 \\
\pi/2 & -0.420 & -0.420 & -1.766 & -1.766 & -1.047 & -1.015 & -0.310 & -0.318 \\
2\pi/5 & -0.914 & -0.366 & -1.707 & -1.707 & -1.089 & -1.089 & -0.460 & -0.349 \\
\end{array}
\]

should be perpendicular to the chain, in contrast to the parallel moment in Co chain. Interestingly, in Cr chain, the antiferromagnetic order is the most stable one, while in Mn chain a chiral order with the \( 2\pi/3 \) period is the lowest energy state. Thus, we do not expect the non-collinear magnetic order as a probable source of the Majorana quasiparticles in Fe and Co magnetic chains.

C. Role of the substrate

Now, we will discuss the results obtained for the chains deposited on a substrate—for the system presented in Fig. 1. In order to simulate the measurements described in Refs. [23] and [49], we take Pb(110) surface as the substrate. To simplify the band structure and make it more readable, in the calculations we have used a system shown in the inset in Fig. 1: containing one transition metal atom and three lead atoms in the unit cell. In the first approximation such a system can help us to describe the influence of neighboring Pb atoms on the transition metal chain.

We start by comparing magnetic moments in the chain. Coupling the chain to the Pb atoms leads to the increase of the magnetic moments only in the case of Cr atom (cf. Tab. I and IV). One should also notice the strong suppression of the magnetic moment in the Co chain.

Deposition of the chains on the substrate changes the system symmetry and allows for the hybridization between the orbitals in the chain and the substrate. These properties lead to the modification of the band structure of the studied system (Fig. 6). To increase the readability of the band structure, the projection of the states into transition metal atoms are shown by colors in the background. From the comparison of the band structures of the isolated chain and the deposited chain, see Figs. 3 and 6, respectively), we can find the influence of the substrate on the chain bands. The bands associated with transition metal atoms have narrower bandwidth with respect to the isolated nanowire. This is equivalent to the modification of the hopping integrals between the atomic orbitals.

Additionally, Fig. 7 presents the density of states (DOS) in the case of the isolated chain (dashed line) and the chain deposited on the substrate (solid line). In the latter case, contributions of the deposited atoms to the total DOS are shown by solid-colored areas. Comparing to the isolated chains, all \( d \)-orbital bands are modified and become narrower. The weakest effect of the substrate is observed for the Fe chain, where the positions of spin-up states very well correspond to those in the isolated chain. Analyzing the electron DOS, we can also explain the modification of the magnetic moments induced by the substrate. In the case of Cr and Mn, the atoms are nearly fully spin polarized (all \( \downarrow \) states are above the Fermi level, while \( \uparrow \) below). In contrast, a small magnetic moment of Co results from the shift of the \( \downarrow \) states to energies below the Fermi level.

Existence of additional bands emerged due to hybridization between the nanowire and substrate makes it impossible for calculations of topological invariant to be carried out. This can have a significant impact in correct description the topological properties of described system and interpenetration experimental results.

Table IV. Magnetic moments (in \( \mu_B \)) in the monoatomic chain deposited on the surface (as shown in Fig. 5).

| atom type | Cr  | Mn  | Fe  | Co  |
|-----------|-----|-----|-----|-----|
| mag. mom. w/ SOC | 2.70 | 2.99 | 2.62 | 0.97 |
IV. SUMMARY

Majorana quasiparticles constitute a very interesting concept of particles, which are indistinguishable from their antiparticles. One of the many platforms in which we expect the emergence of bound states with such properties are systems of magnetic atomic chains deposited on a surface of the conventional superconductor [16–19].

Previous studies of 3d transition metal chains were based on the tight binding models of the bulk systems. Unfortunately, such an approach does not correctly describe the physical properties of the free–standing chains (Sec. IIIA). This is mainly associated with the different distance between atoms in the bulk and the chain, which leads to the modification of the band structure (i.e., hopping integrals between orbitals). We have shown that in the case of isolated chains, the additional band crossing the Fermi level exists, which cannot be captured by the tight binding model obtained from the bulk electronic structure. In consequence, the calculations based on the bulk tight binding models can lead to incorrect conclusions regarding the existence of a non–trivial topological phase in such systems.

To improve the theoretical description of the studied systems, we found the tight binding models in the Wannier orbital basis, stemming from the DFT calculations in the Bloch basis. Using this model we calculated the topological quantum number for isolated nanochains. From the obtained results, we conclude that, in case of isolated nanowires, the non–trivial topological phase can exist only in Mn and Co chains.

Next, we have shown that the non-collinear magnetic order is unstable in the case of the Fe and Co chains (Sec. IIIB). This result may be expected due to strong ferromagnetic instabilities in the bulk Fe and Co [98, 99]. These transition metals demonstrate that the existence of Majorana zero modes in the magnetic chains cannot be considered as a consequence of the non-collinear magnetic order in the chain. Instead, we suggest that it occurs when the number of electrons is even as in Mn or Co, while is absent for an odd electron number. Moreover, the existence of strong magnetic moments in 3d transition metals cannot be correctly captured within the single-band model. On the contrary, this phenomenon is associated not only with Hund’s exchange in partly filled 3d orbital states [98, 99] but also with larger number of bands crossing the Fermi level.

We also discussed the role of the substrate on the monoatomic chains, overlooked in many studies (Sec. IIIC). The interplay between the atoms of the substrate and the chains leads to strong modifications of the electronic properties of the chains. It is clearly visible in the band structure projected onto the chain atoms, as...
as in the density of states. This behavior should be more carefully studied to improve the description of electronic states of the chains deposited on substrates and to better understand the topological properties of these systems.

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