Non-Majorana zero energy modes in diluted spin chains proximitized to a superconductor

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Spin chains proximitized with superconducting condensates have emerged as one of the most promising platforms for the realization of Majorana modes ¹–⁶. The recent use of atomic manipulation techniques raised great expectations for successfully creating and controlling such chains ⁷–¹⁰. Here, we craft diluted spin chains atom-by-atom following seminal theoretical proposal suggesting indirect coupling mechanisms as a viable route to trigger topological superconductivity ³. We demonstrate that, starting from deep Shiba states, it is possible to cross the quantum phase transition, a necessary condition for the emergence of topological superconductivity, for very short chains. This transition is associated with the emergence of highly localized zero energy end modes. The use of a substrate with highly anisotropic Fermi surface enables to create spin chains characterized by distinct magnetic configurations along
various crystallographic directions. By scrutinizing a large set of parameters we reveal the ubiquitous existence of zero energy boundary modes. Although mimicking signatures generally assigned to Majorana modes, the end modes are identified as topologically trivial Shiba states. These results highlight the important role of the local environment, showing that it cannot be completely eliminated also in diluted systems where the effect is expected to be minimized. Our work demonstrates that zero energy modes in spin chains proximitized to superconductors are not necessarily a link to Majorana modes while simultaneously identifying new experimental platforms, driving mechanisms, and test protocols for the determination of topologically non trivial superconducting phases.

Introduction

The development of topological concepts in condensed matter systems has motivated much interest in the realization of Majorana states $^{11,12}$. These exotic states are predicted to emerge at boundaries of topological superconductors $^{13}$, manifesting themselves as zero energy modes in conductance measurements $^{4–8,14,15}$. Beyond their fundamental interest, which illustrates how topological condensed matter systems can be extremely fertile in establishing strong connections with concepts developed in the world of high energy physics $^{16,17}$, the associated non-Abelian exchange statistics has raised great expectations for their direct application in topological quantum computational schemes $^{18}$. Following Kitaev’s seminal proposal $^{19}$, several distinct platforms have been theoretically proposed for their experimental realization, most notably the proximitization of a conventional $s$-wave superconductor to allow for spin-split states, such as by hosting them on topological
insulators\textsuperscript{20}, namely semiconductors with strong spin-orbit coupling\textsuperscript{21,22}, or via magnetic nanostructures\textsuperscript{1–3}.

Since Majorana fermions are a direct manifestation of a topologically non-trivial superconducting state, they are expected to reveal themselves as boundary excitations. For these reasons, spatially resolved spectroscopic techniques are especially suitable to atomically resolve the emergence of Majorana states and to disentangle them from spurious and topologically trivial zero-bias states\textsuperscript{4–6,15,23}. In this context, scanning tunneling microscopy and spectroscopy measurements play a critical role. Following earlier works on self-assembled magnetic chains\textsuperscript{4–6}, the recent use of atomic manipulation techniques has allowed for the construction of disorder-free chains, which has provided insights into the creation and the manipulation of Majorana states\textsuperscript{7–9,24}.

For the building blocks of the Majorana hosting wires, several theoretical proposals have highlighted the important role of impurities with deep Yu-Shiba-Rusinov (YSR, or Shiba) states, i.e. in-gap pairs energetically very close to the Fermi energy, which can undergo a quantum phase transition into a topologically non-trivial superconducting regime even at moderate hybridization strengths\textsuperscript{3}. Moreover, a rich phase diagram was predicted for the realization of Majoranas states using diluted magnetic concentrations with the superconducting host playing an active role in indirectly coupling the impurities\textsuperscript{25,26}. Despite the appealing prospects of the proposed concepts and scenarios, their experimental realization has remained elusive and largely unexplored. Indeed, all systems explored so far are densely packed and ferromagnetically coupled through direct magnetic exchange\textsuperscript{4–9}. 
Here, we use atomic manipulation techniques to create dilute spin chains, where Shiba bands are generated by indirect coupling mediated by the superconducting condensate \(^{27,28}\). We demonstrate that the presence of YSR pairs very close to the center of the superconducting gap allows one to cross the quantum phase transition, a necessary but not sufficient condition for the creation of topologically non-trivial superconducting phases \(^{1-3}\), for relatively short chains. This transition is associated with the emergence of zero-energy modes that are highly localized at the ends of the chains for a large variety of parameters such as coupling strengths, magnetic configurations, and hopping amplitude, and distinct unit cell. Despite hosting spectroscopic signatures typical of Majorana bound states, the end modes are identified as topologically trivial Shiba states energetically pinned at zero. Our results highlight the important role of the local environment even for diluted chains, where it is expected to be minimized, demonstrating how topologically trivial states can effectively mimic signatures generally assigned to Majorana fermions.

**Results**

**Creation of zero energy boundary modes** One dimensional spin chains are created atom-by-atom utilizing atomic manipulation in a STM operated at cryogenic temperatures. Details on sample preparation and measurement protocols can be found in Methods. We focus on Cr atoms indirectly coupled through the (110) surface of niobium, a system which has recently been demonstrated to allow for the tuning of interactions by actively using the superconducting condensate to mediate indirect coupling among the localized Cr spins \(^{28}\). By contrast with atomic chains created by self-assembly, the use of direct atomic manipulation allows for much greater flexibility since it
makes it possible to vary several key experimental parameters such as: (i) chain length, (ii) crystallographic direction, and (iii) distance between local magnetic moments. Despite considerable progress in the field, earlier studies focused on densely packed spin chains, where atoms are nearest neighbors and their coupling is dominated by ferromagnetic direct magnetic exchange $^4$-$^9$, $^{24}$.

Figure 1 reports the creation and spectroscopic characterization of spin chains built atom-by-atom along the crystallographic direction $[1 \bar{1} 3]$. As illustrated in panel a, the distance between successive ad-atoms amounts to 0.55 nm. Figure 1b illustrates the spectroscopic characterization of the atomically crafted chains for representative chain lengths up to 10 atoms. All spectroscopic measurements have been acquired using a superconducting tip, resulting in a convoluted spectrum of tip and sample superconducting energy gaps, $\Delta_{\text{tip}}$ and $\Delta_{\text{sample}}$, where zero energy corresponds to the tip superconducting energy gap (see black dashed line). More spectroscopic data can be found in Supplementary Notes 1-3.

A rich spectroscopic scenario is visible by positioning the STM tip on top of a single Cr ad-atom (N=1) $^{29}$. Several peaks emerge within the bare Nb substrate superconducting energy gap. These peaks are direct fingerprints of magnetic impurity-superconductor interactions, with magnetic moments inducing YSR quasi-particle resonances residing inside the superconducting energy gap. YSR states always appear in pairs that are energetically particle-hole symmetric with respect to the Fermi level $^{30}$-$^{33}$. Their energy is directly linked to the strength of the exchange coupling with the superconducting condensate $J$ while the difference in electron- and hole-like intensity is related to the magnetic impurity being in a spin-screened or free-spin regime. As demonstrated in
Figure 1: Building a chain of Cr atoms, atom-by-atom. a Illustration of the positions of the Cr atoms (red) on the Nb lattice. Atoms are added sequentially along the [1\overline{1}3] direction at a spacing of 0.55 nm; b dI/dU signal measured after sequentially adding Cr atoms to the chain, one atom at a time, up to a chain that is 10 atoms long. For chains longer than N=6 up to 10 atoms, no significant changes in the energy dependence of dI/dU are observed (see Supplementary Information 3 for more data). Black and red signals correspond to the center and end of the chains, respectively. A clear zero bias peak emerges at the chain ends starting from N=3, whose spatial distribution is highly localized, as shown in c. d Energy resolved dI/dU intensity for N=10 visualizing the appearance of highly localized zero-energy modes (see red arrows) located at ±\Delta_{tip} and highlighted in e after subtracting the background inside thebulk of the chains and considering the tip superconducting gap.
Supplementary Note 2, mapping their spatial distribution allows one to clearly identify their orbital character. In the present case, the $d_{z^2}$ orbital dominates near the Fermi level, corresponding to a deep YSR state. This layout represents an ideal situation for the creation of topological superconductivity. When the magnetic impurities are brought close to one another, the YSR states undergo a shift depending on the interaction between adatoms, with the individual YSR states hybridizing and creating the so-called Shiba bands. Since the $d_{z^2}$-derived YSR states are very close to zero energy ($\pm \Delta_{\text{tip}}$ in our case because of the use of superconducting tips), a small hybridization is already sufficient to drive a quantum phase transition where the electron- and hole- component of YSR pairs cross through zero. This quantum phase transition (QPT) is a necessary but not sufficient condition for the transition into a topologically non-trivial superconducting regime where zero-energy modes are trapped and localized at the end of the chain.

Here we scrutinize in more detail the creation and evolution of Shiba bands atom-by-atom starting from the isolated atom case. Spectroscopic results are summarized in Fig.1b. When two adatoms are brought close to each other (N=2), their interaction shifts YSR pairs towards higher binding energies as compared to the single adatom case (N=1). Their spectrum shows higher intensity above the Fermi level, signaling the occurrence of a quantum phase transition. This picture changes when a third atom is added (N=3). Note that N=3 is the smallest possible chain hosting a bulk and an edge. While the energy of the highest intensity YSR state remains unchanged with respect to the N=2 case for the middle atom, which corresponds to the bulk, spectral weight at zero energy is trapped at the end of the chain (red curve). This becomes more evident by progressively increasing the length of the chain. The YSR bands in the bulk (center of the chain)
do not show any significant spectral evolution, within the limit of our experimental resolution, for chains longer than N=6 atoms, signaling that the asymptotic limit is reached for a very short distance. The spatial distribution of the zero-energy mode is reported in Fig.1c. This shows a very strong localization 1 nm, which is independent of the chain length. The localization at the chain ends is also visible in the full spectroscopy map acquired along the chain, reported in Fig.1d. This effect is directly linked to the indirect nature of the coupling between local spins, where the low hopping term giving rise to highly localized end-modes \(^3\). A slightly higher intensity and energy shift is visible for the peak located at \(-\Delta_{\text{tip}}\), a consequence of the stronger background in the bulk of the chains. When this is subtracted and the superconducting tip taken into accounts, this results in a clear zero-bias peak centered at zero, as visualized in Fig.1e. As illustrated in Supplementary Figure 3, not any significant change is observed on longer chains and by using different microtips. This signature is compatible with one of the distinct fingerprints of Majorana modes. Moreover, the persistence of these modes at zero energy independently from the chain length allows us to effectively identify them as boundary modes. However, it is highly unlikely that such short chains realize a topological superconductor, an observation which indicates that they are boundary states, plausibly of trivial origin, and accidentally located at zero. Indeed, it is conventionally expected that at such short distances Majorana states hybridize and split.

**Crystallographic direction and hopping dependence of boundary modes.** The electronic structure anisotropy of the Nb(110) surface \(^{35}\) together with the presence of deep YSR pairs \(^{29,34}\) offers a unique opportunity to experimentally scrutinize different experimental scenarios. Indeed, spin chains built along various crystallographic directions are characterized by distinct spacing among
the atoms, resulting in different interaction strengths and magnetic ground states and, consequently, topological phase diagram (see supplementary information). Moreover, by varying the inter-atomic spacing inside the chain, it is possible to experimentally vary the hopping amplitude. Overall, this supplies unprecedented flexibility to controllably explore the formation of YSR bands in a large experimental parameter space. To shed light on these aspects, Figure 2 displays chains consisting of five atoms aligned along three distinct crystallographic directions, as schematically illustrated in Figure 2a. The inter-atomic spacing is 0.66 nm, 0.57 nm and 0.93 nm along [001], [111] and [110] directions, respectively.

Figure 2b-d shows the spectroscopic mapping of the superconducting state induced in each one of the chains. Its inspection reveals that, despite each direction being characterized by distinct spectroscopic signatures, all chains are characterized by a significant spectral weight accumulation at zero energy localized at the end already for very short chains, as visible in figure 2e-g.

This scenario can be directly controlled by acting on the hopping amplitude, which determines the bandwidth of the Shiba bands. Indeed, for bandwidths smaller than the energy of the single atom YSR pairs, the resulting Shiba bands are well-separated, i.e. electron- and hole-components avoid crossing each other at zero energy, and the system is in a trivial superconducting regime. This concept is illustrated in Fig.2e-g for chains assembled along the [111] direction, i.e. the direction characterized by the smallest possible discrete distance between adatoms. These chains correspond to the experimental realization of the distinct configurations illustrated in the bottom panel of Fig.2a. By increasing the distance between the adatoms (from e to g), the hopping
Figure 2: Spin chains along different directions. a Illustration of the Cr atom positions (red) on the Nb lattice for three different alignments (top panel) and four different spacing between adatoms (bottom panel). In each case a green line shows the connections between the atoms. b-d Spectroscopic mapping of the chain for each of the scenarios illustrated in (a). e-g Highlight the accumulation of spectra weight at zero energy localized at the chains end. All chains consist of five atoms. h-j Spectroscopic mapping of spin chains by progressively increasing the spacing between adatoms.
amplitude is progressively reduced. Our results reveal that, in agreement with expectations, the strong accumulation of spectral weight predominantly localized at the end of the chains becomes very weak for distances of approximately 1.45 nm. Interestingly, a distinct boundary behavior at zero-energy is also found in the metallic regime (see Supplementary Note 5 and discussion below).

Dimerized chains To scrutinize the origin of the zero-energy end modes, we experimentally assembled chains where the unit cell consists of two adatoms. Despite its importance in clarifying the origin of the end modes, this scenario has never been explored so far, with all previous works focusing on chains consisting of equally spaced nearest neighboring adatoms. As schematically illustrated in Figure 3a, a two-atom unit cell structure is achieved by periodically placing adatoms at two distinct distances corresponding to two distinct hopping amplitudes. Fig. 3b shows a topographic image of the resulting spin chain, which consists of 10 unit cells assembled using 20 atoms. The spectroscopic measurements visualize a rather delocalized state with a stronger accumulation of spectral weight at zero-energy localized at the chain end (see the zero energy map and its relative line profile). Its localization still takes place on a very short length scale (see zero energy maps in Figure 3). To clarify the origin of the zero energy modes, we tested their robustness against perturbations. This is illustrated in Figure 3c-d. Figure 3c shows a chain where an additional adatom is placed inside the bulk that acts as a structural and electronic defect, acting as a domain wall. If the zero energy spectral intensity highly localized at the end of the chain would be a Majorana mode, we might expect to observe four: two at the chain ends, and two more on the right and on the left of the domain wall, because the domain wall would cut the topological superconductors
Figure 3: Distinct unit cells and robustness against perturbations. 

**a** Schematic illustration of a two-atoms unit cell spin chain. **b-d** Topography (top panels), zero energy spatial map (middle panels), and spectroscopic mapping (bottom panels) for **b** the pristine chain, **c** chain with internal perturbation, **d** chain with perturbation at the end. Zero energy end modes are visible for all chains. However, a more complex scenario cannot be excluded. Indeed, the chain end and the domain wall are not fully equivalent cases. The defect provides a perturbation as well as a continuity in the electronic structure, which makes it distinct with respect to the chain end. In Figure 3 **d**, additional single adatoms have been connected to the end of the chains. The spectral weight accumulation at zero energy remains localized at the chain end. However, a higher spectral intensity at zero is now observed on both the dimer and the last adatom. Since the bulk of the wire has not been modified, which dictates the topological properties and the intrinsic spatial extension of possible Majorana modes, their localization should not be altered by changing the edge.
**Magnetism, topological invariant and origin of zero energy boundary modes.** In the following we explore theoretically whether the investigated chains can host topological phases. Such a study is currently not accessible from full first-principles simulations and therefore we follow a combined approach. We first address the magnetic and electronic ground-state properties from **ab-initio.** Then we utilize a tight-binding approach parametrized from density functional theory and establish the directional phase diagrams for the infinite wires along the [001], [1\(\bar{1}0\)], [1\(\bar{1}3\)] and [1\(\bar{1}1\)] directions. Finally, we build up a minimal tight binding model to assess the most probable nature of the experimentally unveiled zero energy boundary modes.

Due to the large distances between the Cr atoms in all chains, we find negligible boundary effects in the electronic and magnetic ground-state structures of the chains. The magnetic moments of approximately 3.0 \(\mu_B\) per atom are uniformly distributed with a difference of less than 0.02 \(\mu_B\) between the edge and the central atoms for all chains. The different chains exhibit fundamentally different magnetic exchange interactions among nearest neighboring adatoms, ranging from antiferromagnetic coupling of \(J = 2.1\) meV for the [1\(\bar{1}0\)] chain and \(J = 11.5\) meV for the [001] chain to ferromagnetic coupling of \(J = -6.2\) meV for the [1\(\bar{1}1\)] chain and \(J = -1.7\) meV for the [1\(\bar{1}3\)] chain. Minimizing a Heisenberg model with the magnetic exchange parameters from first principles leads to the ground states of the chains shown in Figure 4a. Due to the weak Dzyaloshinskii-Moriya interaction, the chains are almost collinear and follow the ferro- and antiferromagnetic couplings dictated by the isotropic exchange (see Methods section and Supplementary Note 6 for more details).
**Figure 4:** Topological properties and magnetic ground states of the different Cr chains deposited on the Nb(110) surface. Shown are the [001], [1T3], [1T1], and [1T0] directions. 

**a** Magnetic structures obtained from first principles (see Methods). 

**b** Phase diagrams of the Majorana number for the infinite wires as function of the spin splitting $U$ and the energy of the $d$-orbitals $E_d$. Topological regions are shown in blue, while the trivial non-topological regions are white. For more details see Supplementary Note 5.

After assessing the magnetic behavior of the wires, we establish a map of the topological invariant for all chains shown in Figure 4b. This is realized via an effective multi-orbital tight-binding model utilizing parameters obtained from first-principles in the metallic regime and...
including the proximity-induced superconductivity as a parameter. We explore the topological behavior by varying the exchange splitting and the energy of d-orbital. Starting from weak hopping and corresponding flat bands, such as those present in the [101] chain, topologically trivial and non-trivial regions are well separated. The non-trivial regions are defined by thin stripes that depend on the crystal field splitting of the Cr atoms and the chain direction, which influences the orbital character of the hopping. Increasing the hopping amplitude increases the bandwidths and thus the topological non-trivial regions, as can be seen in the [111] and [131] chains. This effect continues for the [001] chain, where the hopping is comparable to crystal field splitting, leading to an overlap of the different bands and a complex phase diagram. The spatial range of the hopping is paramount in designing the topological character of the wires.

Figure 4b uses a hopping up to the first four neighbors, which can influence the formation of topological regions in the phase diagram in a constructive or a destructive way depending on the details of the hopping. For example, the non-trivial regions are amplified by considering four neighbors instead of only nearest neighbors for the [001] chain, while they are reduced in size for the [101] chain.

Our model gives key insight into understanding which are the key parameters that govern the transition into a topological non-trivial regime, and highlights the crucial role of electronic hoping in its experimental realization, independently from the magnetic state. Owing to the presence of multiple white stripes of different widths, the phase diagrams illustrate that the realization of topological superconducting phases is not straightforward. When the complexity of real materials is
taken into account, it requires fine tuning of several parameters such as hopping amplitude, multi-orbital nature and magnetic interactions.

To shed light onto the appearance of the zero-energy modes, we numerically examine different spin chains by utilizing a minimal tight binding model; the details of the model are described in Supplementary Note 8. In particular, we consider the trivial regime by neglecting the spin-orbit interaction (SOI). For a single magnetic impurity, the experimental data reveal a deep YSR state close to zero energy (see Supplementary Note 2). This occurs for a certain exchange coupling strength \( J = J_c \), which we fix in our model, unless stated otherwise. Adding further nearby magnetic impurities leads to hybridization and energy splitting of the YSR states as a function of their overlap, which is determined by the distance \( L \) between the impurities. If the impurities are deposited close to each other, e.g. only separated by one lattice spacing, the energy of the lowest sub-gap state strongly oscillates as a function of the chain length, as shown in Fig. 5a. For specific chain lengths, the lowest energy state can be experimentally detected as a zero-energy mode if the finite energy resolution is taken into account. Moreover, the probability density of the lowest sub-gap state and the local density of states (LDOS, which accounts also for higher states due to the finite-energy broadening \( \epsilon \)) are both characterized by large weights on the ends of the chain, as illustrated in Fig. 5d.

Next, we consider well-separated impurities at a distance \( L = 5a \) to simulate the experimental scenario scrutinized in the present study, i.e. the indirectly coupled regime. In this case,
Nearst neighbour adatoms | Indirectly coupled adatoms | SSH Chain

Figure 5: Energies and wave functions for different impurity chain configurations. The adatoms are separated by a distance (a, d) $L = a$ and (b, e) by $L = 5a$. (c, f) The impurities are ordered in unit cells: each unit cell contains two adatoms. We set the intra unit cell distance between the two adatoms to $L = a$ and the spatial separation between the unit cells to $L = 4a$. Forty lowest energies (a, b) as a function of the number of impurities $N$ and (c) as a function of the number of unit cells $N_u$. (d-f) Probability density and LDOS at zero energy at the cross-section of the chain. The parameters used for the figure are $t = 1$, $\Delta = 0.2$, $\mu = 1$, $\epsilon = 0.01$ and the total size is $N_x \times N_y = 50 \times 92$. Furthermore, we used $J = J_c \approx 2.47$ in panels (a, b, d, e) and $J = J_c \approx 1.88$ in panels (c, f).

The splitting is much weaker and the resulting YSR band appears narrow and localized around zero energy, as shown in Fig. 5b. In other words, the system hosts states with almost zero energy.
independent of the length of the chain. For some parameter choices the probability density of the lowest sub-gap state along the chain reveals large weights even on the ends of the chains, see Fig. 5e, matching the experimental observation (see Fig. 1 and Fig. 2). Being the YSR states in the model energetically close to each other, we calculate the LDOS with a broadening parameter $\epsilon$ to account for the finite experimental energy resolution. The LDOS reveals, similar to the probability density, large peaks at the ends of the chain (see Fig. 5e), effectively reproducing the experimental observations. Therefore, without claiming that the experimental situation is exactly captured by the minimal tight binding model, we conclude that trivial mechanisms can lead to effects similar as those observed in the experiments.

Finally, we order the impurities in unit cells. In particular, two impurities are separated by one lattice spacing $a$ in each unit cell and the unit cells are separated by a distance of $L = 4a$. In order to find trivial zero-energy states, we start by calculating the energies of a system consisting of one unit cell as a function of the exchange coupling strength. The two overlapping YSR states have zero energy at $J_<$ and $J_>$, respectively, with $J_< < J_c < J_>$. Finally, we set the exchange coupling strength to $J_<$ and calculate the energies as a function of the number of unit cells $N_u$. The unit cells are well separated and a narrow band forms around zero energy, as shown in Fig. 5c. The probability density of the lowest state has again strong weights on the ends of the chain and the LDOS (see Fig. 5f) looks similar to the experimental $dI/dV$ zero-energy map reported in Fig. 3b. We would like to note that the effect of having a higher intensity at the end is not generally valid for the probability density of the lowest state, i.e. for other chain lengths the weight can be distributed differently. However the LDOS, which takes multiple states close to zero energy into account, has
almost the same shape also for varying chain length, namely peaks at the positions of the unit cells at slightly higher peaks at the ends of the chain.

Conclusion

Our results systematically scrutinize dilute spin chains proximitized to a superconducting condensate. Contrary to earlier studies on ferromagnetically coupled and densely packed adatoms\(^4\)\(^-\)\(^9\), our platforms effectively uses the superconducting condensate as an active element to mediate the interaction between adatoms. Starting from single adatoms hosting deep Shiba states, we demonstrate the ability to create distinct magnetic ground state configurations hosting Shiba bands crossing the Fermi level. This is associated to the emergence of highly localized zero energy boundary modes showing some spectroscopic signatures in agreement with expectations for Majorana modes. However, these are identified as trivial Shiba states characterized by a larger spectral weight localized at the chain ends. Our results implies that zero bias, length independent, boundary modes are not necessarily a link to Majorana modes. At the same time, by using indirectly coupling mechanisms on anisotropic surfaces, we demonstrate that it is possible to significantly enlarge the experimental parameter space, opening new routes for the experimental search of topologically non-trivial superconducting states.

Methods

**Sample and tip preparation.** A clean Nb(110) substrate was obtained by flashing the crystal to 2300 K in 12 s\(^37\) hundreds of times. Measurements were taken at a temperature T = 600 mK
using the Tribus STM head ( Scienta Omicron). Cr adatoms were deposited in-situ using an e-beam evaporator while keeping the sample below a temperature of 15 K. All atoms were found to be adsorbed in the hollow site of the Nb(110) surface \(^{38}\). Cr chains have been assembled by atomic manipulation technique by dragging them with the STM tip in constant current mode using a setpoint of \(V = -5 \text{ mV} \); \(I = 70 \text{ nA} \). \(dI/dU\) spectra were acquired by standard lock-in technique.

To enhance the energy resolution, we used superconducting Nb tips obtained by deep indentations into the Nb single crystal.

**First-principles and tight-binding model calculations** The ab-initio simulations are based on the scalar-relativistic full-electron Korringa-Kohn-Rostoker (KKR) Green function augmented self-consistently with spin-orbit interaction \(^{39,40}\). The theoretical framework uses multiple-scattering theory allowing an embedding scheme, which is ideal to address the electronic and magnetic properties of nanostructures in real space without the use of periodic supercells. We utilize the atomic-sphere approximation (ASA) and consider the full charge density within the local spin density approximation (LSDA) \(^{41}\). We assume an angular momentum cutoff at \(\ell_{\text{max}} = 3\) for the orbital expansion of the Green function and when extracting the local density of states a k-mesh of \(150 \times 150\) is considered. The Nb(110) surface is modelled by slab containing 22 layers enclosed by two vacuum regions with a thickness of 9.33 Å each. Due to the large spacings between the atoms of the Cr chains we use the geometrical properties obtained for isolated Cr adatoms. Thus, the chain atoms are placed on the hollow stacking site relaxed towards the surface by 20% of the inter-layer distance of the underlying Nb(110) surface, which was shown to be the energetically favoured stacking for isolated adatoms in Ref. \(^{38}\).
To describe the magnetic structure of the chains we use the generalized Heisenberg model,
\[
H = \sum_i e_i \mathcal{K}_i e_i + \frac{1}{2} \sum_{ij} J_{ij} e_i \cdot e_j + \frac{1}{2} \sum_{ij} D_{ij} \cdot (e_i \times e_j) ,
\]
where $\mathcal{K}_i$ is the on-site anisotropy, $J_{ij}$ is the isotropic exchange interaction and $D_{ij}$ is the Dzyaloshinskii-Moriya interaction between the $i$-th and $j$-th atom with the magnetic moment $m_i = m_i e_i$. The magnetic exchange interactions were obtained using the magnetic force theorem in the frozen-potential approximation and the infinitesimal rotation method. The on-site magnetic anisotropy of the Cr atoms in all chains is obtained from the method of constraining fields, and was found to be similar to the one of the isolated adatoms reported in Ref. Further information can be found in Supplementary Note 4.

The topological invariant is calculated using a tight-binding model with parameters obtained from density functional theory and an effective Hamiltonian construction (see Ref. and Supplementary Note 6).

**Authors contributions** S.L. and P.S. conceived the project. F.K. performed the STM measurements and analysed the experimental data under supervision of S.S.P. and P.S.. S.B. performed the ab-initio simulations. S.B. and S.L. conceived the mapping approach from first-principles to tight-binding and studied the related computed data. R.H, D.L. and J.K developed the minimal tight-binding model, performed simulations and analysed the associated results. P.S. wrote the initial version of the manuscript to which all authors contributed.

**Competing Interests** The authors declare that they have no competing interests.

**Data and materials availability** All data needed to evaluate the conclusions in the paper are present in
the paper and/or the supplementary materials. Additional data related to this paper may be requested from
the authors. The KKR Green function code that supports the findings of this study is available from the
corresponding author on reasonable request.

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