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Topological and trivial domain wall states in engineered atomic chains

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In a recent article[1], Huda et al. demonstrated tuneable topological domain wall states in the $c(2\times2)$ chlorinated Cu(100)[2]. Their system allows to experimentally tune the domain wall states using atom manipulation by the tip of a scanning tunneling microscope (STM). They have realized topological domain wall states of two prototypical one-dimensional models such as trimer[3] and coupled dimer chains[4–8]. However, they did not distinguish trivial domain wall states[9] from topological ones in their models. As a result, all states of a specific domain wall are not topological but trivial. Here, we show why the specific domain wall states are trivial and how to make them topological. This topological consideration would provide more clear insight into future studies on topological domain wall states in artificial atomic chains.

Before discussing the topology of domain walls, we need to introduce an important constraint in the coupled dimer chains as follows. A coupled dimer chain consists of two interacting Su-Schrieffer-Heeger (SSH) chains that connect each other via the zigzag interchain coupling (dashed lines in Fig. 1). Since each SSH chain undergoes a period-doubling charge-density-wave (CDW) transition through the Peierls dimerization at low temperature, a coupled dimer chain also exhibits the Peierls dimerization. The equilibrium atomic displacement ($\pm\Delta_0$ in Fig. 1, up to 10% of the undimerized atomic spacing[10,11]) is determined by the balance between the electronic energy gain due to the CDW gap opening and the elastic energy cost due to the Peierls dimerization. When we construct any topological domain walls in coupled dimer chains, we keep in mind that they should be able to be undimerized within reasonable atomic displacements. This constraint guarantees that there are no structural defects such as vacancies or extra atoms in topological domain walls.

However, the previously-reported domain wall structure (Fig. 1a) has a single vacancy when it is undimerized. In addition, its characteristic zigzag interchain coupling is also missing at the domain wall. Due to such imperfections, we cannot properly discuss its topology. Furthermore, the domain wall is not topological without considering the constraint because both upper and lower SSH chains are topologically trivial (see below). To rectify these imperfections, we simply modify the domain wall by including the 'missing' atom (Fig. 1b).

In the SSH model, the topological invariants or Zak phases[12] of dimer chains depend on the ratio between intradimer (t) and interdimer (t') hopping parameters. The Zak phase, θ_{Zak}, can be obtained through the Bloch wave functions $|u_k\rangle$: $\theta_{\mathrm{Zak}} = \mathrm{i}\int_{-\pi/2a_0}^{\pi/2a_0}\langle u_k|\partial_k u_k\rangle\, dk$, where a_0 is the lattice period of the undimerized chain. A ground state shows $\theta_{\mathrm{Zak}}=0$ (blue region in Supplementary Fig. 1a) when $|t/t'|>1$ while $\theta_{\mathrm{Zak}}=\pi$ (red region in Supplementary Fig. 1b) when $|t/t'|<1$. Due to the bulk-boundary correspondence, topological domain wall states emerge at the interface between topologically distinct Zak phases while we do not expect any topological edge states between the topologically same Zak phases. Such topological domain wall states depend only on topology of ground states but not the strength of hopping parameters[9]. As shown in Supplementary Fig. 1c, d, both domain wall states do maintain their topology even though trivial edge states appear at higher hopping parameters.

By coupling two SSH chains, we introduce a coupled dimer chain with four ground states where topological chiral domain wall states can emerge when one of two SSH subchains has an interface between topologically distinct Zak phases[5–8]. However, the defective domain wall AA → AB (Fig. 1a) proposed by Huda et al. actually does not have any topological edge mode because both the upper and lower SSH chains exhibit the same trivial topology (Supplementary Fig. 1e). In contrast, the corrected domain wall AA → AB (Fig. 1b) has a topological edge mode at the lower chain (Supplementary Fig. 1f).

Based on our topological consideration, we perform the tight-binding calculations as Huda et al. did[1] to compare two structurally and topologically different domain walls. As shown in Fig. 2a, b, two domain wall configurations exhibit distinct energy spectra. Most notably, all domain wall states (black dots) are trivial in Fig. 2a while a topological domain wall state (red dot) emerges in the upper band gap in Fig. 2b. We confirm that such domain wall states are adiabatically connected to non-interacting SSH chains without interchain coupling (as we described above) as well as that some trivial domain states appear under the strong interchain coupling (Supplementary Fig. 2).

Furthermore, we check the spatial localization of these domain wall states by plotting the simulated local density of states (LDOS) maps as shown in Fig. 2d–f. Whereas the trivial domain wall state is localized at the upper chain with no phase shift ($\theta_{\mathrm{Zak}}=0\rightarrow0$, Fig. 2d), the topological state mainly exists at the domain wall site on the lower chain with the distinct topology shift ($\theta_{\mathrm{Zak}}=0\rightarrow\pi$, Fig. 2e). In addition, the topological domain wall state only shows characteristic alternating zero LDOS next to the domain wall just like SSH topological solitons[10,13]. Such topological properties are also observed in another chiral domain wall AA → BA reported by Huda et al. (Fig. 2c, f). Note that Fig. 2b, c now exhibit the topologically opposite chirality, which has been reported in other systems[5,6,8].

We showed why the original domain wall configuration is not topological and the new configuration has the topological domain wall state. However, the new configuration is impossible to realize on the chlorinated Cu(100) because the domain wall should be located in between chlorine sites. Instead, we propose an alternative configuration (Supplementary Fig. 3) with the same topology, which requires higher energy cost. Thus, we can

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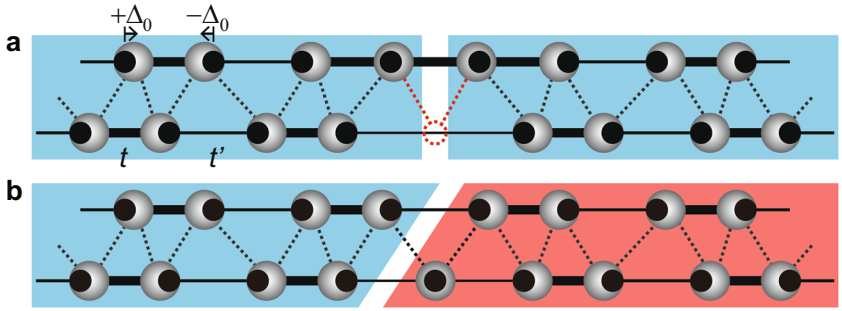

Fig. 1 Schematics of topologically distinct domain walls in coupled dimer chains. a, **b** Atomic models of domain wall structures **a** with and **b** without a single vacancy. Red dotted circle and lines represent a missing atom and its interchain coupling that Huda et al. did not consider in their model. Undimerized (dimerized) atoms in the chains are indicated by black (gray) circles. $\pm\Delta_0$ denote the equilibrium dimerization displacements with respect to the undimerized phase. Here, $\Delta_0 = 0.1a_0$ is the same value as Huda et al. used[1], where a_0 is the undimerized atomic spacing. t and t' indicate intradimer and interdimer hopping parameters, respectively. Blue (red) shaded background means trivial (nontrivial) ground states.

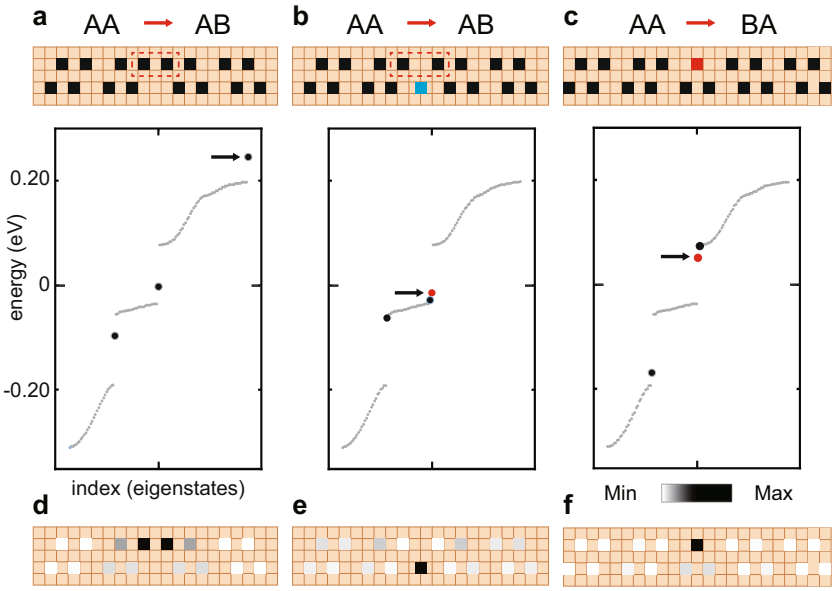

Fig. 2 Topological and trivial domain wall states in coupled dimer chains. a–**c** Atomic configurations and corresponding energy spectra of domain walls: **a**, **b** AA → AB and **c** AA → BA. The atomic configurations in **a** and **b** have the same domain walls as Fig. 1a, b, respectively. Red dashed rectangles indicate the difference on the upper chains between **a** and **b**. Red, black, and gray dots in the energy spectra represent topological, trivial domain wall states, and bulk states, respectively. **d**–**f** Simulated local density of states (LDOS) maps of **a**–**c** at the energy levels indicated by black arrows in **a**–**c**. Black (white) denotes the highest (lowest) LDOS.

experimentally access both topological and trivial domain states because they now exist below the conduction band of the chlorine layer[1].

Although Huda et al. have demonstrated various tuneable topological domain wall states using atom manipulation, they have not properly considered the atomic and topological structures. As a result, one of the domain wall configurations proposed by Huda et al. does not have any topological edge mode due to the atomic vacancy and is inconsistent with their other topological domain walls. To overcome this inconsistency, we suggested the alternative domain wall configuration without defects leading to a topological domain wall state. Our analysis would be corroborated by topological invariants of chiral domain wall states, which requires further investigation beyond our scope. Such careful topological considerations will provide further insight on topological domain wall states in any artificial atomic chains.

DATA AVAILABILITY

The data sets generated and/or analyzed during the current study are available from the corresponding author on reasonable request.

CODE AVAILABILITY

The custom codes generated and/or analyzed during the current study are available from the corresponding author on reasonable request.

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AUTHOR CONTRIBUTIONS

S.-G.J. and T.-H.K. conceived the idea, carried out the calculations and the analyses, and wrote the manuscript.

COMPETING INTERESTS

The authors declare no competing interests.

ADDITIONAL INFORMATION

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