Supplementary Information:
Topological and trivial domain wall states in engineered atomic chains

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FIG. S1. Atomic schematics of 1D domain walls. a Schematic model of an SSH chain having two identical domain walls. Ground states can have either $A$ ($|t/t'| > 1$) or $B$ ($|t/t'| < 1$) phases. Red atoms represent domain walls connecting one ground state to the other. b, c Atomic configurations on the chlorinated Cu(100) of a. Black and red/blue squares (chlorine vacancies) denote bulk and domain walls, respectively. Two red domain walls connect $A$ to $A'$ in b while red and blue domain walls do $A$ to $A$ in c. d Schematic model of coupled dimer chains having two opposite chiral domain walls. Two domain walls (indicated by red and blue atoms) topologically annihilate each other. e, f Atomic configurations on the chlorinated Cu(100) of d. In e, an initial ground state $AA$ is transformed into a somewhat different ground state $A''A''$ by using two domain walls Huda et al. proposed. In contrast to e, a ground state returns to itself via two chiral domain walls in f. Note that the blue domain wall cannot be experimentally realized on the chlorinated Cu(100) (see Fig. S3).
**FIG. S2.** Adiabatic evolution of topological and trivial domain wall states. **a,b** Energy diagrams as a function of the interchain coupling ($t_I$) of Fig. 2a,b. Red and black lines indicate topological and trivial domain wall states, respectively, while gray shaded regions denote bulk states. Such adiabatic evolution maintains topology of domain wall states regardless of the interchain coupling strength. The left and right ends represent Fig. 2 in the main text and ones without the interchain coupling, respectively.

**FIG. S3.** Experimentally feasible AA–AB domain wall. **a** Proposed AA → AB domain wall in Fig. 2b of the main text. **b** Alternative AA → AB domain wall for experimental realization by adding more spaces between two ground states. Red dashed rectangles highlight the difference of the upper chains between **a** and **b**. Tight-binding calculations give similar energy spectra and confirm these two configurations are adiabatically connected (or topologically the same). Furthermore, the topological domain wall state exists in the band gap, which is experimentally accessible because it is much lower than the conduction band of the chlorine layer.
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In a recent article, Huda et al. demonstrated tuneable topological domain wall states in the c(2×2) chlorinated Cu(100). 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 1D models such as trimer and coupled dimer chains. However, they did not distinguish trivial domain wall states 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 on future studies on topological domain wall states in artificial atomic chains.

First, we point out a limitation of the discrete atomic lattice: artificially designed ground states do not respect the symmetry of target models. For example, in the Su–Schrieffer–Heeger (SSH) model, due to their $Z_2$ symmetry, one ground state should be transformed to the other and then return to the initial ground state via two successive identical SSH domain walls ($A → B → A$) (Supplementary Fig. 1a). However, the same transformation cannot be realized for the chlorinated Cu(100) (Supplementary Fig. 1b). If we use the same domain wall structure twice, then we end up with a different ground state ($A'$) from the initial one ($A$). To correct this discrepancy, we need to introduce a somewhat different domain wall configuration indicated by the blue square in Supplementary Fig. 1e.

Thus, this corrected atomic configuration does not fully respect the SSH symmetry because two domain walls are not identical like the SSH model.

In a similar way, we consider the coupled dimer chain consisting of two coupled 1D dimerized chains. Because two opposite chiral domain walls (red and blue dots in Supplementary Fig. 1d) on the same chain can annihilate each other, one ground state can return to itself ($A A → B A → A A$). However, due to the limitation of the discrete atomic lattice, one ground state cannot come back to the initial ground state ($A A → B A → A' A''$, Supplementary Fig. 1e) by using opposite chiral domain walls proposed by Huda et al. To rectify this contradiction, we suggest another domain wall configuration that includes an additional atom (blue square in Supplementary Fig. 1f).

Next, we discuss the topology of domain wall states in 1D chain systems. In the SSH model, the topological invariants or Zak phases of dimer chains depend on the ratio between intra-dimer ($t$) and interdimer ($t'$) hopping parameters. The Zak phase, $\theta_{Zak}$, can be obtained through the Bloch wave functions $|u_k\rangle$: $\theta_{Zak} = i \int_{-\pi/a_0}^{\pi/a_0} \langle u_k | \partial_k u_k \rangle dk$, where $a_0$ is the lattice period of the dimer chain. As shown in Fig. 1a,b, a ground state shows $\theta_{Zak} = 0$ when $|t/t'| > 1$ (red regions) while $\theta_{Zak} = \pi$ when $|t/t'| < 1$ (a blue region). Topological domain wall states emerge at the interface between topologically distinct Zak phases ($\theta_{Zak} = 0 ↔ \pi$, Fig. 1b,d) while we do not expect any topological edge states between the topologically same Zak phases ($\theta_{Zak} = 0 ↔ 0$, Fig. 1a,c).

Such topological domain wall states depend only on topology of ground states but not the strength of hopping parameters. In other words, adiabatic deformation of Hamiltonians does not change the topology of domain wall states. Therefore, all Hamiltonians are said to be adiabatically equivalent or adiabatically connected when we continuously tune the hopping parameters $t_a$ and $t_b$ at domain walls by maintaining the system's symmetry (Fig. 1a,b). As shown in Fig. 1c,d, both domain wall states do maintain their topology even though trivial edge states appear at higher hopping parameters at the domain walls ($|t_{a,b}| > \min(|t|, |t'|)$).

In this sense, the domain wall $AA → AB$ (Fig. 1e) proposed by Huda et al. actually does not have any topological edge modes because the upper and lower chains exhibit the same trivial topology such as Fig. 1a. In contrast, the domain wall $AA → AB$ (Fig. 1f) suggested by us indeed do have a topological edge mode at the lower chain.

Based on our topological consideration, we perform the tight-binding calculations as Huda et al. did to compare two different domain walls. As shown in Fig. 2a,b, two domain...
Fig. 2. **Topological and trivial domain wall states in coupled dimer chains.** a–c Atomic configurations and corresponding energy spectra of domain walls: $AA \rightarrow AB$ (a,b) and $AA \rightarrow BA$ (c). The atomic configurations in a and b have the same domain walls as Fig. 1e and f, 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.

Wall configurations exhibit distinct energy spectra. Most notably, all domain wall states (black dots in Fig. 2a) are trivial in the domain wall Huda et al. proposed while a topological domain wall state (red dot in Fig. 2b) emerges in the upper band gap in our domain wall configuration. We confirm that such domain wall states are adiabatically connected to ones without interchain coupling as well as some trivial domain states appear under the strong interchain coupling as described in 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 where there is no phase shift ($A \rightarrow A$, Fig. 2d), the topological state mainly exists at the domain wall site on the lower chain where there is the distinct topology shift ($A \rightarrow B$, Fig. 2e). Such topological properties are also observed in another chiral domain wall state $AA \rightarrow BA$ reported by Huda et al. (Fig. 2c,f). Note that Fig. 2b and c now exhibit the topologically opposite chirality, which has been reported in other systems.

Although the authors have demonstrated various tuneable topological domain wall states using atom manipulation, they have not properly considered topology. As a result, one of the domain wall configurations proposed by Huda et al. does not have any topological edge mode and is inconsistent with their other topological domain walls. We suggested the alternative domain wall configuration, which recovers a topological domain wall state regardless of the interchain coupling. Such careful topological considerations will provide further insight on topological domain wall states in any artificial atomic chains.

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