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MATTERS ARISING OPEN



Reply to: “Topological and trivial domain wall states in engineered atomic chains”

Md Nurul Huda¹, Shawulienu Kezilebieke^{1,2}, Teemu Ojanen^{3,4}, Robert Drost¹ and Peter Liljeroth¹✉REPLYING TO: Seung-Gyo Jeong and Tae-Hwan Kim *npj Quantum Materials* <https://doi.org/10.1038/s41535-022-00424-y> (2022)*npj Quantum Materials* (2022)7:23; <https://doi.org/10.1038/s41535-022-00425-x>

Topological modes in one- and two-dimensional systems have been proposed for numerous applications utilizing their exotic electronic responses. Su-Schrieffer-Heeger (SSH) model–one-dimensional (1D) dimer chain—is one of the simplest models exhibiting topological states. While the edge modes in the SSH model are exactly at the mid-gap energy, other paradigmatic 1D models such as trimer and coupled dimer chains have non-zero energy boundary states. In our original paper¹, we realized atomically controlled trimer and coupled dimer chains using chlorine vacancies in the $c(2 \times 2)$ adsorption layer on Cu(100)². This built on earlier work on atomically controlled dimer chains³, where the desired structures are fabricated using atom manipulation by low-temperature scanning tunneling microscopy (STM).

The comment by Seung-Gyo Jeong and Tae-Hwan Kim concentrates on one particular domain wall (DW) structure formed in the coupled dimer chain system. They identify limitations imposed by the discrete atomic lattice in realizing structures where we go through the different dimerization states of the atomic chains (e.g. AA \rightarrow BA \rightarrow AA). They show theoretically that the domain wall AA \rightarrow AB suggested by us does in fact not have topological DW states and propose an alternative structure that would indeed have them. The new domain wall structure is the “opposite” to our AA \rightarrow BA domain wall that has a topological state also according to the analysis by Jeong and Kim. We agree with their analysis and thank them for investigating this in detail and highlighting the difference between idealized models and atomic scale systems, where the discrete lattice has to be taken into account.

While the domain wall states can be readily detected using STM and scanning tunneling spectroscopy (STS), this comment highlights the need to develop experimental methods to identify topological invariants in atomic scale systems from local measurements and to distinguish topological from trivial domain wall states. In both cases, small changes of system parameters or external fields will only give rise to a small variation of the DW states: they are not moved to the continuum, i.e. the resulting states can be robust towards small perturbations. Of course, the topological DW states are protected towards arbitrary perturbations if the special symmetry, which protects the topology remains intact.

It will be interesting to realize the new proposed domain wall structures experimentally and develop methods for extracting the topological invariants from measurements of the local density of states (LDOS) using STM and STS^{4,5}. These atomically well-defined systems can also serve as a platform for developing these methodologies.

DATA AVAILABILITY

All relevant data are available from the authors upon request.

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AUTHOR CONTRIBUTIONS

T.O. and P.L. discussed the content of this reply and P.L. wrote the reply, M.N.H., S.K. and R.D. read and agreed to this reply.

COMPETING INTERESTS

The authors declare no competing interests.

ADDITIONAL INFORMATION

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