
This is an electronic reprint of the original article.
This reprint may differ from the original in pagination and typographic detail.

Huda, Md Nurul; Kezilebieke, Shawulienu; Ojanen, Teemu; Drost, Robert; Liljeroth, Peter
Reply to: "Topological and trivial domain wall states in engineered atomic chains"

Published in:
npj Quantum Materials

DOI:
[10.1038/s41535-022-00425-x](https://doi.org/10.1038/s41535-022-00425-x)

Published: 16/02/2022

Document Version
Publisher's PDF, also known as Version of record

Published under the following license:
CC BY

Please cite the original version:
Huda, M. N., Kezilebieke, S., Ojanen, T., Drost, R., & Liljeroth, P. (2022). Reply to: "Topological and trivial domain wall states in engineered atomic chains". *npj Quantum Materials*, 7(1), 1-2. Article 23.
<https://doi.org/10.1038/s41535-022-00425-x>

This material is protected by copyright and other intellectual property rights, and duplication or sale of all or part of any of the repository collections is not permitted, except that material may be duplicated by you for your research use or educational purposes in electronic or print form. You must obtain permission for any other use. Electronic or print copies may not be offered, whether for sale or otherwise to anyone who is not an authorised user.

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.

Received: 30 June 2021; Accepted: 13 January 2022;
Published online: 16 February 2022

REFERENCES

1. Huda, M. N., Kezilebieke, S., Ojanen, T., Drost, R. & Liljeroth, P. Tuneable topological domain wall states in engineered atomic chains. *npj Quantum Mater.* **5**, 17 (2020).
2. Kalf, F. E. et al. A kilobyte rewritable atomic memory. *Nat. Nanotechnol.* **11**, 926–929 (2016).
3. Drost, R., Ojanen, T., Harju, A. & Liljeroth, P. Topological states in engineered atomic lattices. *Nat. Phys.* **13**, 668–671 (2017).
4. Carvalho, D., García-Martínez, N. A., Lado, J. L. & Fernández-Rossier, J. Real-space mapping of topological invariants using artificial neural networks. *Phys. Rev. B* **97**, 115453 (2018).
5. Caio, M. D., Caccin, M., Baireuther, P., Hyart, T. & Fruchart, M. Machine learning assisted measurement of local topological invariants. Preprint at <https://arxiv.org/abs/1901.03346> (2019).

ACKNOWLEDGEMENTS

We acknowledge funding from European Research Council (ERC-2017-AdG no. 788185 “Artificial Designer Materials”), Academy of Finland (Academy professor funding no. 318995 and 320555, and Academy research fellow no. 338478).

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

Correspondence and requests for materials should be addressed to Peter Liljeroth.

Reprints and permission information is available at <http://www.nature.com/reprints>

Publisher's note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.

¹Department of Applied Physics, Aalto University School of Science, PO Box 15100, FI-00076 Aalto, Finland. ²Department of Physics, Department of Chemistry and Nanoscience Center, University of Jyväskylä, FI-40014 University of Jyväskylä, Jyväskylä, Finland. ³Computational Physics Laboratory, Physics Unit, Faculty of Engineering and Natural Sciences, Tampere University, PO Box 692, FI-33014 Tampere, Finland. ⁴Helsinki Institute of Physics, PO Box 64, FI-00014 Helsinki, Finland. ✉email: peter.liljeroth@aalto.fi



Open Access This article is licensed under a Creative Commons Attribution 4.0 International License, which permits use, sharing, adaptation, distribution and reproduction in any medium or format, as long as you give appropriate credit to the original author(s) and the source, provide a link to the Creative Commons license, and indicate if changes were made. The images or other third party material in this article are included in the article's Creative Commons license, unless indicated otherwise in a credit line to the material. If material is not included in the article's Creative Commons license and your intended use is not permitted by statutory regulation or exceeds the permitted use, you will need to obtain permission directly from the copyright holder. To view a copy of this license, visit <http://creativecommons.org/licenses/by/4.0/>.

© The Author(s) 2022