

==== response to referee 1 ====

We thank the referee for their careful reading of our manuscript and their helpful remarks. We are glad that the referee appreciates both our findings and the way we present them. We will address the remarks of the referee point by point below, indicating the referee's comments in *red*, and our responses in *blue*.

1)

- *this is a very well-written paper*
- *the splitting into main text/appendices is appropriate, and the latter provide many useful details on the authors' results*
- *the results are general and apply in a model-independent way*
- *I believe this work will lead to multiple follow-up theoretical and experimental investigations*

[..]

- *I really enjoyed reading this paper, it is very well written. Results are presented in a step-by-step pedagogical way, making the authors' discussion easy to follow also for non-specialists. I think this work is timely and of interest to the community working on topological systems, and it will motivate experimental studies on these kinds of interface states, possibly in various meta-material platforms.*

We thank the referee for these endorsements of our work.

2)

- *it would really help the readers to see one simple example Hamiltonian showing the behavior discussed in the paper.*

[..]

- *Please add an example. I understand that the work is general, and that the results apply in a model-independent way: this is one of the strengths of the paper. However, it would really help the readers to have something concrete to point to while going through these general results. With even a simple example in an appendix somewhere, I believe the quality of this paper would be greatly improved.*

We thank the referee for insisting on this point.

This same suggestion was also made by referee 2, and in an independent comment by Dr. Varjas. Although beyond the scope of the original work, we agree that an explicit example strengthens the presentation in the paper, and will help to clarify some of the formal results. We therefore constructed not one, but two explicit examples and include a detailed discussion of these in a new section added to the revised manuscript.

One example is particularly intuitive, being a 2D extension of the well-known SSH model. The other, based on a 2D extension of 1D CDWs, is slightly less familiar, but conceptually cleaner as it does not include any chiral symmetries. Both examples give the same results in terms of interface states, in complete agreement with the predictions arising from the theory described in the earlier sections.

The new section also includes an analysis of the effect of impurities at the interface, which we discuss in more detail below.

3)

Several times throughout the paper, but especially at the beginning of Section 4, the authors refer to interface states which should be present at the Fermi level. At the end of Section 5, the authors say that these interface states may sensitively depend on crystal terminations. This makes me confused with respect to the way in which the authors define "topological protection."

My confusion is as follows:

As far as I can understand (again, here an example would go a long way), the symmetry labels force interface-bound states to exist, but they don't force these states to continuously interpolate

in energy between the valence and the conduction band. My naive guess (which could be wrong) is that these states exist at some particular energy, which is in general different from 0 since there is no chiral or particle-hole symmetry in class A. The interface between two inversion-symmetric bulks is in general not inversion-symmetric, so it might be possible to change the microscopic details of the interface without worrying about inversion breaking. In this case, isn't it possible for me to freely move these interface states in energy, simply by changing the microscopic details of the interface itself? For instance, could I add a chemical potential just to the interface, and push the interface states up in energy until they overlap with the bulk bands?

We thank the referee for clearly formulating this issue. We agree that in hindsight, we did not sufficiently clearly define what we mean by "topological protection". This is clarified in the revised manuscript, both in the introduction and discussions sections, and (by explicit example) in the newly added section.

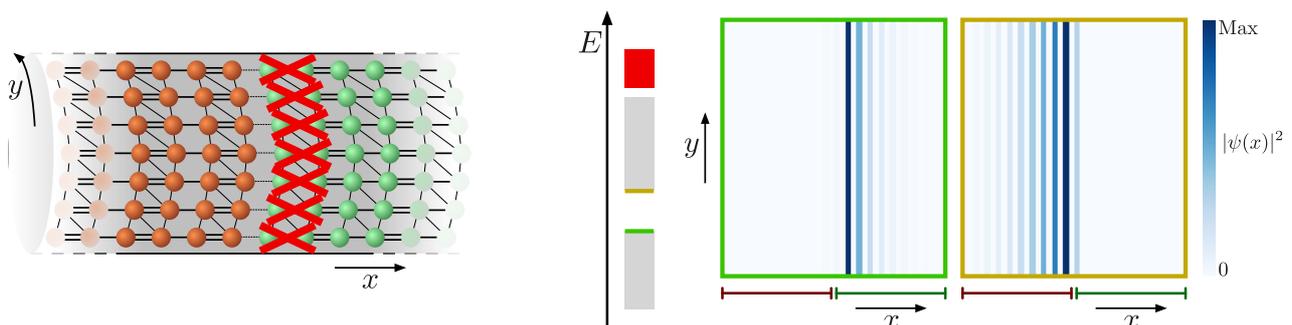
We believe there are two related issues to be clarified regarding this point. First of all, one may ask about the question of existence of interface states. Here, the prediction is clear: as long as the lattice symmetry is respected and the band gap does not close, topological states must exist in a gap between atomic insulators sharing the same sign of the logarithmic derivative. In the new section with examples, we indeed find all of the predicted interface states in both of the models we discuss. The existence of these states is guaranteed by the symmetry labels of the bands, and in that sense "protected" by lattice symmetry.

Then, there is the question of the energies at which topological interface modes appear, and how these may be influenced. Here, the referee is correct that there is no reason for the states to appear in the middle of the gap, and the states do not connect any bulk bands. This is expected for states arising from a weak invariant, and different from topological states associated with non-zero net Berry curvature. It indeed also makes it possible for added potentials to alter the energies of the interface states.

In the new section we show the explicit example of a very strong impurity potential (exceeding the bulk bandwidth) being added at the interface. This can be clearly seen to create a local, non-topological impurity state at high energy, and to suppress the weight of the topological interface states at the impurity site (figure 5 of the revised manuscript). The wavefunction of the topological interface state away from the impurity site is not affected, however, and the wave functions does in particular still span the entire interface. It is therefore not destroyed by the presence of even a very strong impurity and can be employed in practice even in the presence of (strong) impurities.

Moreover, we also studied the case of adding a strong impurity potential (with a strength comparable to the bulk band width) across the entire interface. These results are not included in the revised manuscript, both because this situation is unrealistic and because the results are somewhat counter-intuitive. However, we do present them in the figure below.

Upon adding a potential across the entire interface, the band of interface states can be moved arbitrarily close towards the bulk band, as the referee suggested. For very high impurity potential a band of states localised at the impurity (i.e. at the interface) appears on top of the entire spectrum — these are the red states in the spectrum of the second panel below, which should be compared to the red interface state in figure 5 of the revised manuscript. However, these impurity states are not the topological interface states, which can still be discerned within the bulk gap, but arbitrarily close to the bulk band. In the figure below, these are the green and brown states localised at the edges of the band gap. Plotting their real-space wave functions (rightmost panels)



clearly shows these states to be the interface states, split into two parts and displaced away from the impurity potential, but still exponentially localised at the interface.

The topological interface states thus do enjoy some form of topological protection, in the sense that they must exist in the gap and cannot be destroyed or brought into the bulk. But the energy at which they occur can in principle (with unrealistic impurity potentials) be brought arbitrarily close to the gap edges.

4)

Note that this would be very different from the "topological protection" of strong TIs (e.g. quantum spin-Hall effect) and what people used to call weak TIs (e.g. 3D stack of 2D QSHE). In those systems, the boundaries are invariant under the symmetries (time reversal, translation) and the boundary states exist at the Fermi level no matter how one changes the microscopic details of the interface, provided its symmetries are left intact.

As also discussed above, we agree with this difference in the nature of the topological protection for strong and weak topological modes, and we comment on this in the revised manuscript.

The comment of the referee also brings to light the fact that we did not clearly define our use of the terms "strong" and "weak" topological insulators in the original manuscript. We intended for them to follow the standard nomenclature in the classification of topological insulators on the basis of K-theory (which was central to the identification of the symmetry-label-based invariants discussed in this paper). We thank the referee for highlighting this omission, and we added an explicit definition of these terms in the introduction of the revised manuscript.

5)

Are the states discussed in this paper and their amount of topological protection different from Shockley states? Does this paper discuss the conditions for which Shockley states exist in p2, p3, and pmm?

We thank the referee for these questions, which help to clarify the message of our paper.

First of all, we understand "Shockley states" to refer to the edge states of a one-dimensional tight-binding model introduced by Shockley in 1939 (our reference 36 in the revised manuscript). These edge states were generalised by Zak in 1985 (reference 42), using a more universally applicable formalism culminating in a symmetry criterion for the existence of edge states. Both authors considered a clean edge at a high-symmetry point in a one-dimensional chain, and they both considered an interface between the chain and the vacuum, rather than between two crystalline insulators.

In the present work, we extend Zak's symmetry criterion to higher dimensions and to interfaces between crystalline insulators. Moreover, we show the resulting generalised symmetry criterion for the existence of edge states to coincide with the topological criterion established in our Ref. 19. Within the framework of symmetry-label based topology, an interface between crystalline insulators is both more natural and more general than an interface with the vacuum. Our results confirm the topological nature of occupation numbers for bands of a given symmetry, and establishes a bulk-boundary correspondence for them.

Rather than saying that the interface states presented here are merely generalised versions of Shockley states, we thus suggest that rather, Shockley states should be re-interpreted as the simplest possible incarnation of the topological interface states we introduce and examine in the present manuscript.

==== response to referee 2 ====

We thank the referee for their careful reading of our manuscript and their helpful remarks. We are glad that the referee appreciates strength and counterintuitive nature of our findings. We will address the remarks of the referee point by point below, indicating the referee's comments in red, and our responses in blue.

1)

The authors claim that a group of weak topological invariants, which depend only by the symmetries of the atomic lattice, induces a bulk-boundary correspondence.

In particular, it is claimed that (i) these weak topological invariants predict the presence or absence of states localised at the interface between two inversion-symmetric band insulators with trivial values for their strong invariants, and (ii) the interface modes are protected by the combination of band topology and symmetry of the interface.

We thank the referee for the clear summary of our results.

2)

These statements are strong and counterintuitive, and I don't find the supporting arguments in the manuscript convincing. The essential counterargument opposing these statements that it seems likely that it is possible to introduce a perturbation which obeys the symmetries but moves the interface states in energy to the conduction or valence band on either side of the interface. Thus, the interface states hybridise with the bulk states and are no longer localised at the interface. (Notice that the energy gap can be very small on one side of the interface, and therefore intuitively it seems that it would be very easy to hybridize the interface states with the bulk bands on that side of the interface.) This would mean that the interface states are not protected by the combination of the band topology and symmetry of the interface, and therefore also the weak topological invariants would not always predict the presence or absence of localised states at the interface.

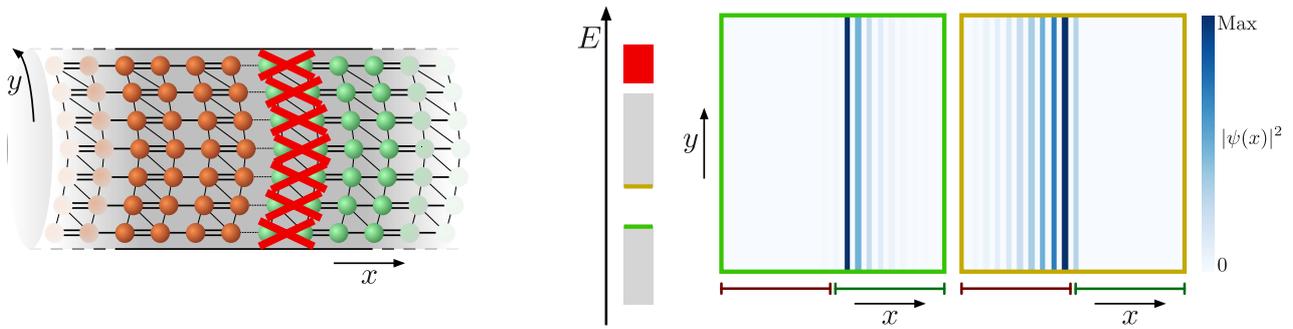
We thank the referee for raising this issue. Part of the confusion about the protection of the edge states may be due us not sufficiently clearly defining what we mean by "topological protection" in the original submission. This is clarified in the revised manuscript, both in the introduction and discussions sections, and (by explicit example) in the newly added section.

Besides the issue of definition, we believe there are two related issues at play, which were also raised by referee 1. We repeat our arguments from the reply to referee 1 here.

First of all, one may ask about the question of existence of interface states. Here, the prediction is clear: as long as the lattice symmetry is respected and the band gap does not close, topological states must exist in a gap between atomic insulators sharing the same sign of the logarithmic derivative. In the new section with examples, we indeed find all of the predicted interface states in both of the models we discuss. The existence of these states is guaranteed by the symmetry labels of the bands, and in that sense "protected" by lattice symmetry.

Then, there is the question of the energies at which topological interface modes appear, and how these may be influenced. Here, the referee is correct that there is no reason for the states to appear in the middle of the gap, and the states do not connect any bulk bands. This is expected for states arising from a weak invariant, and different from topological states associated with non-zero net Berry curvature. It indeed also makes it possible for added potentials to alter the energies of the interface states.

In the new section we show the explicit example of a very strong impurity potential (exceeding the bulk bandwidth) being added at the interface. This can be clearly seen to create a local, non-topological impurity state at high energy, and to suppress the weight of the topological interface states at the impurity site (figure 5 of the revised manuscript). The wavefunction of the topological interface state away from the impurity site is not affected, however, and the wave functions does in particular still span the entire interface. It is therefore not destroyed by the presence of even a very strong impurity and can be employed in practice even in the presence of (strong) impurities.



Moreover, we also studied the case of adding a strong impurity potential (with a strength comparable to the bulk band width) across the entire interface. These results are not included in the revised manuscript, both because this situation is unrealistic and because the results are somewhat counter-intuitive. However, we do present them in the figure below.

Upon adding a potential across the entire interface, the band of interface states can be moved arbitrarily close towards the bulk band, as the referee suggested. For very high impurity potential a band of states localised at the impurity (i.e. at the interface) appears on top of the entire spectrum — these are the red states in the spectrum of the second panel below, which should be compared to the red interface state in figure 5 of the revised manuscript. However, these impurity states are not the topological interface states, which can still be discerned within the bulk gap, but arbitrarily close to the bulk band. In the figure below, these are the green and brown states localised at the edges of the band gap. Plotting their real-space wave functions (rightmost panels) clearly shows these states to be the interface states, split into two parts and displaced away from the impurity potential, but still exponentially localised at the interface.

The topological interface states thus do enjoy some form of topological protection, in the sense that they must exist in the gap and cannot be destroyed or brought into the bulk. But the energy at which they occur can in principle (with unrealistic impurity potentials) be brought arbitrarily close to the gap edges.

3)

It is probably possible to formulate a weaker statement, which is related to statement (i). Namely, I expect that quite generically these weak topological invariants are related to the presence or absence of localised states at the interface. The appearance of such interface states can be understood by first considering a smooth interface with slowly varying parameters connecting the two Hamiltonians, and then realising that one needs quite large perturbation to remove the resulting localised interface states appearing inside the bulk gap. Thus, the interface states will often survive in specific models even in the case of a sharp interface. Nevertheless, I want to emphasise that these localised interface states are not protected just by symmetry and topology; Their appearance requires additional assumptions about the model Hamiltonian.

We appreciate the attempt by the referee to give an alternative interpretation for the results in our manuscript. Although the arguments brought forward by the referee indeed seem intuitive, they do not capture all of the involved physics. In particular, we believe the explicit example discussed above clearly establishes the topological nature of the interface states, in direct agreement with the K-theory-based suggestion in Ref. 19 of the revised manuscript that the occupation numbers of states in given representations at high-symmetry points in the Brillouin zone are, by themselves, *bona fide* (weak) topological invariants.

4)

I am willing to reconsider the paper for publication if the authors have additional arguments to support their statements that the interface states are indeed protected by the combination of band topology and symmetry of the interface. For this purpose I suggest that the authors construct an explicit example (as suggested also both by Daniel Varjas and the first referee), and study the robustness of the interface states with respect to introducing all possible symmetry-preserving perturbations which do not change the band topology.

We thank the referee for their suggestion, which we follow and report on in the new section of the revised manuscript and in our response above.