Abstract Submitted
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Computing topological invariants without inversion symmetry ALEXEY SOLUYANOV, DAVID VANDERBILT, Rutgers University — We consider the problem of calculating the weak and strong topological indices in noncentrosymmetric time-reversal (T) invariant insulators. In 2D we use a gauge corresponding to hybrid Wannier functions that are maximally localized in one dimension. Although this gauge is not smoothly defined on the two-torus,[1] it respects the T symmetry of the system and allows for a definition of the Z_2 invariant in terms of time-reversal polarization.[2] In 3D we apply the 2D approach to T-invariant planes. We illustrate the method with first-principles calculations on GeTe and HgTe under [100] and [111] strain. Our approach is different from the one suggested previously by Fukui and Hatsugai[3] and should be easier to implement in *ab initio* code packages. Time permitting, we will also discuss methods for decomposing the band space into T-paired Chern subspaces, and for carrying out a general construction of a Wannier representation for Z_2 insulators.

[1] A. A. Soluyanov and D. Vanderbilt, arXiv:1009.1415
[2] L. Fu and C. L. Kane, Phys. Rev. B **74**, 195312 (2006)
[3] T. Fukui and Y. Hatsugai, J. Phys. Soc. Jpn. **76**, 053702 (2007)

Alexey Soluyanov
Rutgers University

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