

Title: Pseudo-atomic orbital based tight-binding model investigation of Fermi Arcs in Na₃Bi.

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Na₃Bi is a topological Dirac semimetal [1] whose double surface Fermi arcs were initially thought to be topologically protected [1-3]. Angle resolved photoemission spectroscopy (ARPES) measurements on Na₃Bi's (100) facet [4] are consistent with double surface Fermi arcs [1,2]. However, it was shown that bulk symmetry preserving terms that leave the Dirac points unchanged could deform the double surface Fermi arcs into a closed Fermi contour that does not connect to the Dirac points [5] and could be still consistent with the ARPES data.

We investigate how robust the double surface Fermi arcs are to Na₃Bi (100) slabs with different terminations. We construct tight binding models of two Na₃Bi (100) slabs using pseudo-atomic orbitals [6]. Away from the projected Dirac points we find slab termination localized states. Near the projected Dirac points there is a hybridization of surface and bulk states. Both findings are consistent with the predicted behavior of Fermi arcs in Na₃Bi. We find that while the arcs are not strictly topologically protected, they are quite robust for realistic surfaces.

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1. Z. Wang, et al, Phys. Rev. B 85, 195320 (2012).
2. A. C. Potter, I. Kimchi, and A. Vishwanath, Nature Communications 5, 5161 (2014).
3. E. V. Gorbar, V. A. Miransky, I. A. Shovkovy, and P. O. Sukhachov, Phys. Rev. B 91, 121101 (2015).
4. S.-Y. Xu, et al, Science 347 (2015).
5. M. Kargarian, M. Randeria, and Y.-M. Lu, Proceedings of the National Academy of Sciences 113 (2016).
6. M. Buongiorno Nardelli, et al, Computational Materials Science 143 (2018).