Perfect Topological Metal CrB₂: A One-Dimensional (1D) Nodal Line, a Zero-Dimensional (0D) Triply Degenerate Point, and a Large Linear Energy Range

1. Berry Phase Calculation

To capture the nature of the nodal lines, the Berry phase was computed, where the Berry phase was connected to the occupied Bloch band [1,2]. The result is shown in Figure S1. Obviously, the Berry phase experienced a jump around the nodal line in the $k_z = 0$ plane.
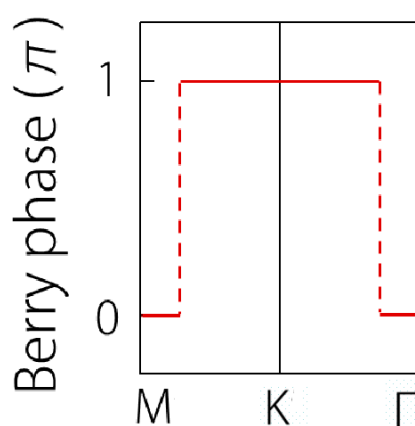

Figure S1. The Berry phase along the M–K–Γ k-path for closed nodal line.

References

1. Wan, X., Turner, A.M., Vishwanath, A., & Savrasov, S. Y. (2011). Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates. *Physical Review B*, 83(20), 205101.
2. Burkov, A. A., Hook, M. D., & Balents, L. (2011). Topological nodal semimetals. *Physical Review B*, 84(23), 235126.