Dual topological insulating phase in NaZnBi

Hyunggeun Lee[*], Yoon-Gu Kang[*], Myung-Chul Jung[*], Myung Joon Han[*†], and Kee Joo Chang[*‡]

[*]Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon 34141, Korea

Email: [†]mj.han@kaist.ac.kr and [‡]kjchang@kaist.ac.kr

Based on first-principles calculations, we report a dual topological insulator (DTI) phase in NaZnBi, which exhibits both topological insulator and topological crystalline insulator phases [1]. NaZnBi was recently synthesized in a PbFCl-type tetragonal structure with *P*4/*nmm* space group [2]. Through Wannier charge center calculations, we find the $\mathbb{Z}_2$ indices $(\nu_0; \nu_1\nu_2\nu_3) = (1; 000)$ and odd mirror Chern numbers $C_{\mathbb{M}} = \pm 1$ in NaZnBi. Furthermore, we confirm that the topological surface Dirac points are maintained even when time-reversal or mirror symmetry is broken due to the robustness of the DTI phase. Therefore, we expect that NaZnBi will be a good candidate for future device applications.

[1] Lee, H., Kang, Y.-G., Jung, M.-C., Han, M. J. & Chang, K. J. Robust dual topological insulator phase in NaZnBi. *NPG Asia Mater.* **14**, 1–8 (2022).

[2] Shilov, A. I., Pervakov, K. S., Tafeenko, V. A. & Morozov, I. V. New Ternary Bismuthides NaZnBi and NaCdBi: Synthesis and Crystal Structures. *Russ. J. Coord. Chem.* **46**, 622–630 (2020).