**Prediction of Large-Gap Topological Insulator in functionalized Ordered Double Transition Metal MXene**

Mei-Ling Xu1,＋ , Zhi-Quan Huang1, Gennevieve Macam1, Chia-Hsiu, Hsu1, Feng-Chuan Chuang1,\*

*1Department of Physics, National Sun Yat-Sen University, Kaohsiung 804, Taiwan*

+Presenter: Mei-Ling Xu, b042030009@g-mail.nsysu.edu.tw

\*Corresponding Author: Feng-Chuan Chuang, fchuang@mail.nsysu.edu.tw

**ABSTRACT**

MXenes have become popular 2D materials in the recent years owing to their various composition and surface functional possibilities. Though numerous MXenes were predicted to possess topological properties [1,2,3], the exploration of topological phase in MXenes is still ongoing. Here, we conduct a rigorous search study on V2TiC2 with various surface terminations, X2(X = F, Cl, I, Br, O, H, and OH) using first-principles calculations. We find that V2TiC2F2 is a topological insulator determined from the calculations of the topological invariant and the parities of wave functions at the time reversal invariant momentum (TRIM) points of the Brillouin zone below the fermi level. It has a non-trivial band gap of 40 meV and 251 meV using GGA and hybrid functionals, respectively. Further analysis shows that majority of the contribution of band inversion are from the *d*-orbitals of V atoms. We also find that V2TiC2F2 remains a robust topological insulator against tensile strain up to 19%. The combined unique properties of topological insulators and MXenes makes it a valuable 2D material worth of further study with a potential to play an important role in the development of technology.

[1] Hongming Weng, Ahmad Ranjbar, Yunye Liang, Zhida Song, Mohammad Khazaei, Seiji Yunoki, Masao Arai, Yoshiyuki Kawazoe, Zhong Fang, and Xi Dai, Large-gap two-dimensional topological insulator in oxygen functionalized MXene. Phys. Rev. B 92, 075436 (2015).

[2] H. Mohammad Khazaei, A. Ranjbar, M. Arai, and S. Yunoki, Topological insulators in the ordered double transition metals M'2M"C2 MXenes (M' = Mo, W; M" = Ti, Zr, Hf). Phys. Rev. B, 94 125152 (2016).

[3] C. Si, K. H. Jin, J. Zhou, Z. Sun, and F. Liu, Large-Gap Quantum Spin Hall State in MXenes: D-Band Topological Order in a Triangular Lattice. Nano Lett. 16, 6584 (2016).