**Prediction of Quantum Anomalous Hall Effect in MBi and MSb (M:Ti, Zr, and Hf) Honeycombs**

Zhi-Quan Huang1, Wei-Chih Chen1, Gennevieve M. Macam1+, Christian P. Crisostomo1, Shin-Ming Huang1, Rong-Bin Chen3, Marvin A. Albao4, Der-Jun Jang1,2, Hsin Lin5,6,7, Feng-Chuan Chuang1,2\*

*1Physics, National Sun Yat-Sen University, Kaohsiung, Taiwan
2Multidisciplinary and Data Science Research Center, National Sun Yat-Sen University, Kaohsiung, Taiwan
3Center of General Studies, National Kaohsiung Marine University, Kaohsiung, Taiwan
4Institute of Mathematical Sciences and Physics, University of The Philippines Los Baños, Laguna, Philippines
5Institute of Physics, Academia Sinica, Taipei, Taiwan
6Centre for Advanced 2D Materials and Graphene Research Centre, National University of Singapore, Singapore, Singapore
7Department of Physics, National University of Singapore, Singapore, Singapore*

+ Presenter:Gennevieve M. Macam, mmgennevieve@gmail.com

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

**Abstract**

The abounding possibilities of discovering novel materials has driven enhanced research effort in the field of materials physics. Only recently, the quantum anomalous hall effect (QAHE) was realized in magnetic topological insulators (TIs) albeit existing at extremely low temperatures. Here, we predict that MPn (M=Ti, Zr, and Hf; Pn=Sb and Bi) honeycombs are capable of possessing QAH insulating phases based on first-principles electronic structure calculations. The application of strain shows that HfBi, HfSb, TiBi, and TiSb honeycomb systems possess QAHE with the largest band gap of 15 meV. In low-buckled HfBi honeycomb, we observed decreasing Chern number with increasing lattice constant. The band crossings occurred at low symmetry points. We found that by varying the buckling distance we can induce a phase transition such that the band crossing between two Hf d-orbitals occurs along high-symmetry point K2. Moreover, edge states are demonstrated in buckled HfBi zigzag nanoribbons. This study contributes additional novel materials to the current pool of predicted QAH insulators which have promising applications in spintronics.

Keywords: Quantum anomalous Hall effect, Topological phase transition, TM-Bi honeycomb, Electronic structures, First-principles calculations