Electronic Supplementary Material (ESI) for Nanoscale.

Large Gap Two-Dimensional Topological Insulators with the coexistence of the Significant Rashba Effect and the Piezoelectricity in Functionalized PbGe Monolayers

Ningyuan Shen, Shuangying Lei*, Yonghu Wang, Neng Wan, Jie Chen, Qinan Huang

[a] Key Laboratory of Microelectromechanical Systems of the Ministry of Education, Southeast University, Nanjing 210096, China.

*Corresponding author. E-mail address: lsy@seu.edu.cn (S. Lei)

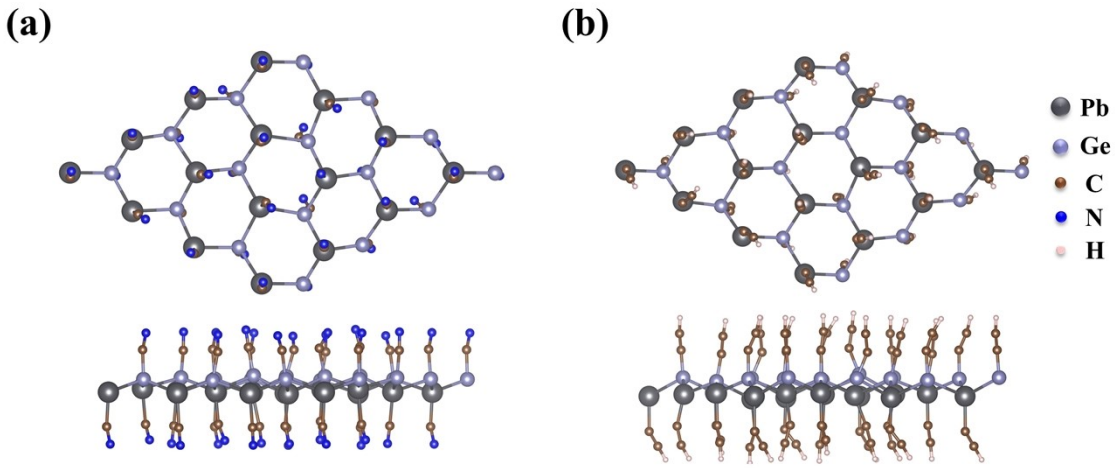

Figure S1. Top and side view of the structures of (a) $PbGe(CN)_2$ and (b) $PbGe(C_2H)_2$ after 4ps of the MD simulation at 300 K with NVT ensemble.

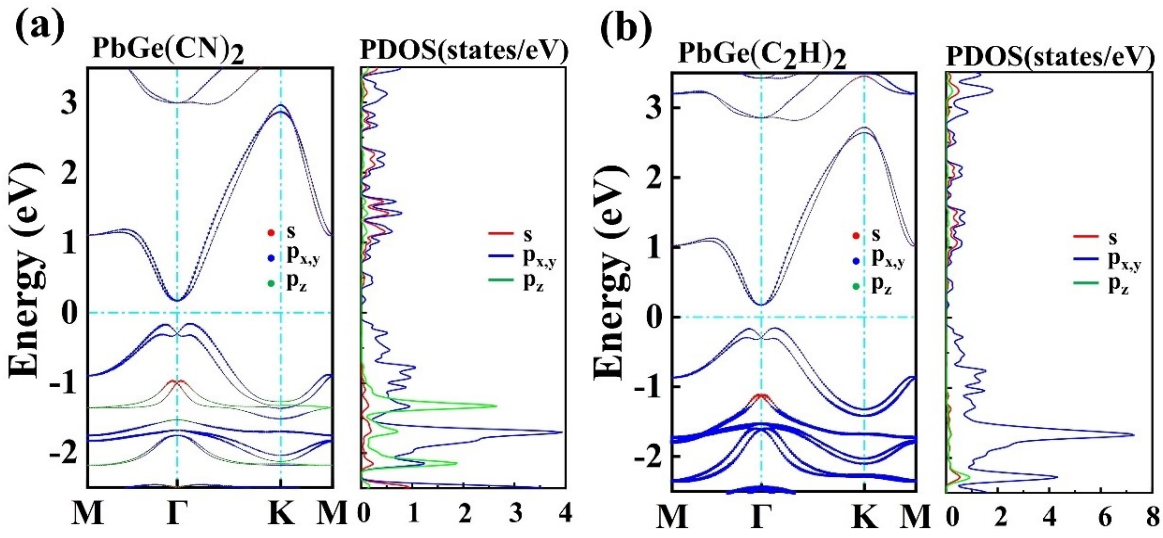

Figure S2. The projected density of states (PDOS) for $PbGe(CN)_2$ and $PbGe(C_2H)_2$.

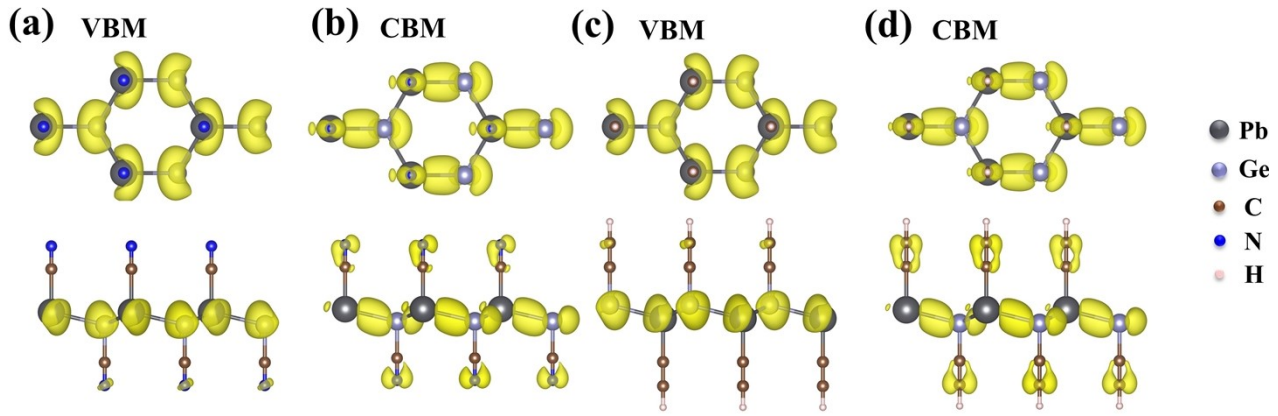

Figure S3. The partial charge density (PCD) of VBM and CBM for $PbGe(CN)_2$ and $PbGe(C_2H)_2$.

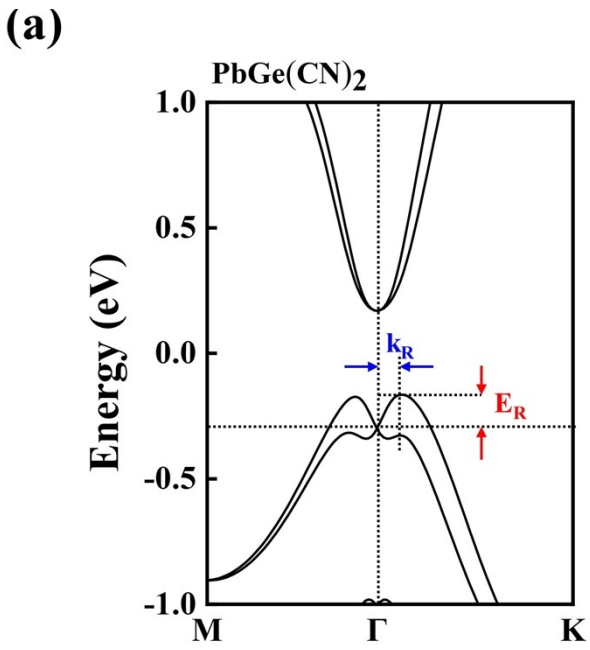

Figure S4. The schematic diagram of Rashba splitting energy E_R and momentum offset k_R.

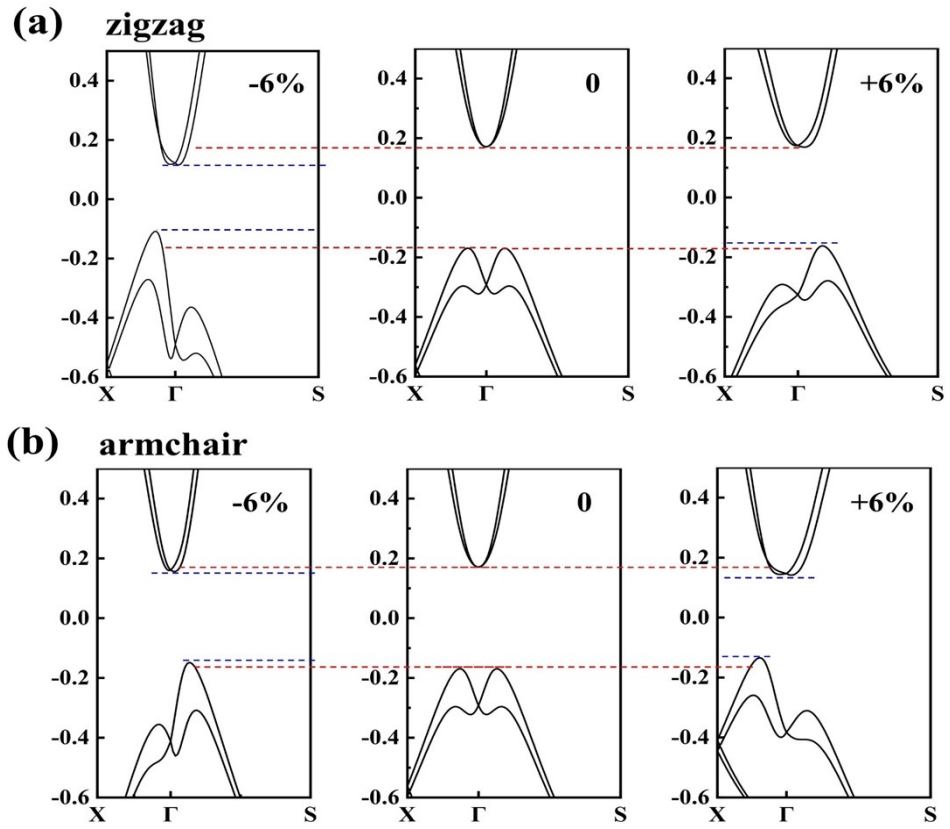

Figure S5. The variation trend of the VBM and CBM under uniaxial strain along the (a)zigzag direction and (b) armchair direction for $PbGe(C_2H)_2$.

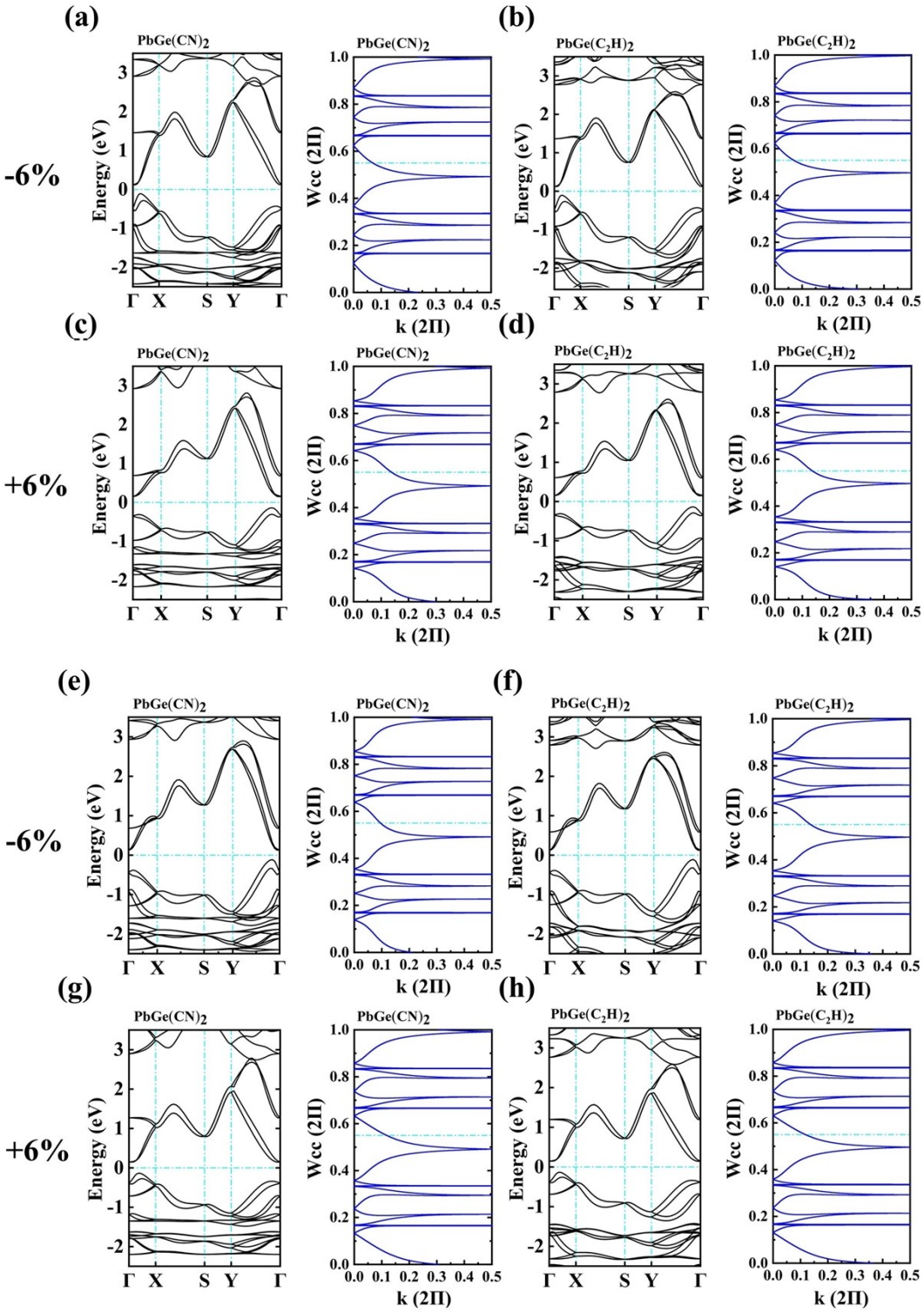

Figure S6. The band structures and WCCs evolutions at the uniaxial strain of -4% and 6% along the (a-d) zigzag direction and (e-h) armchair direction.