Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Possibility of regulating valley-contrasting physics and nontrivial topology by ferroelectricity in functionalized arsenene

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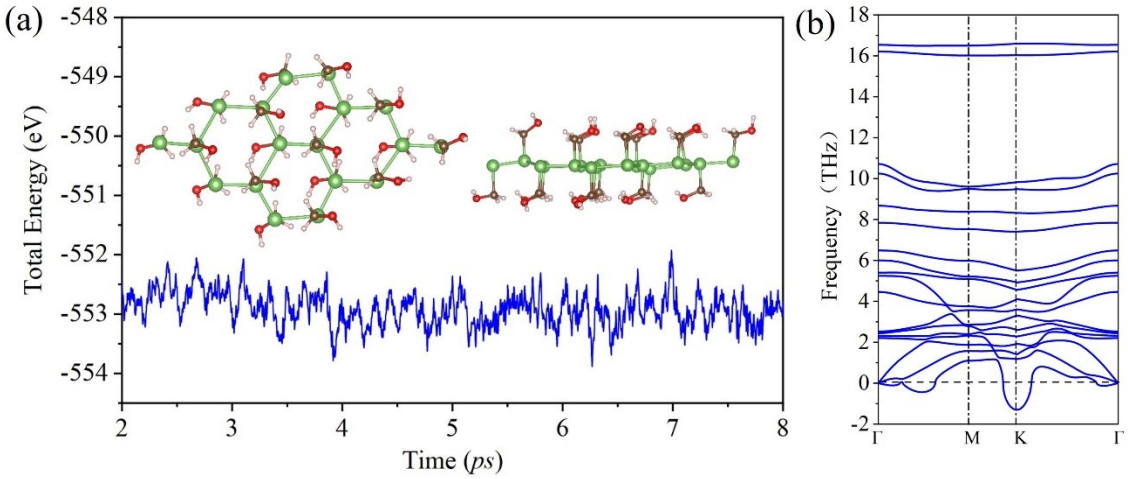

Fig. S1 (a) Evolution of the total energy for the monolayer A-AsCH_2OH obtained from the AIMD simulation at 237K. The inset is the final structure of the monolayer A-AsCH_2OH. (b) Calculated phonon spectrum of the monolayer A-AsCH_2OH.

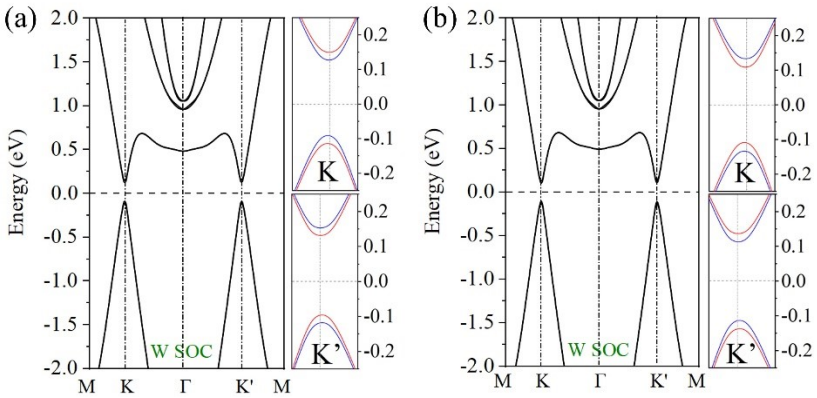

Fig. S2 Calculated band structure based on HSE06 functional for monolayers A-AsCH_2OH (a) and A'-AsCH_2OH (b).

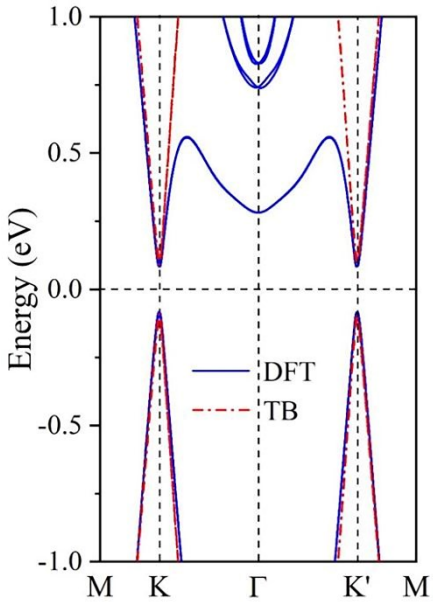

Fig. S3 Band structure of the monolayer A-AsCH$_2$OH obtained from DFT calculation and TB fitting.

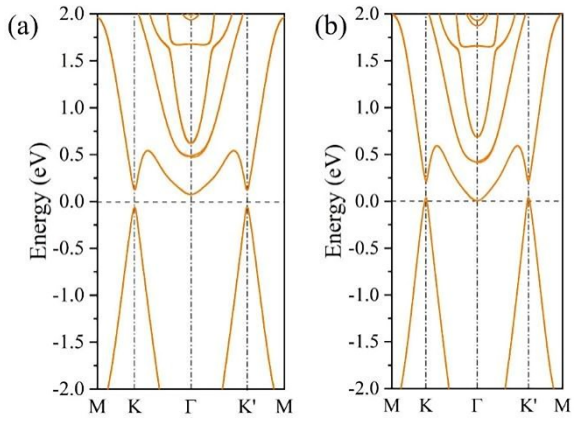

Fig. S4 Band structure of the monolayer A-AsCH$_2$OH with 3% (a) and 4% (b) compressive strain.

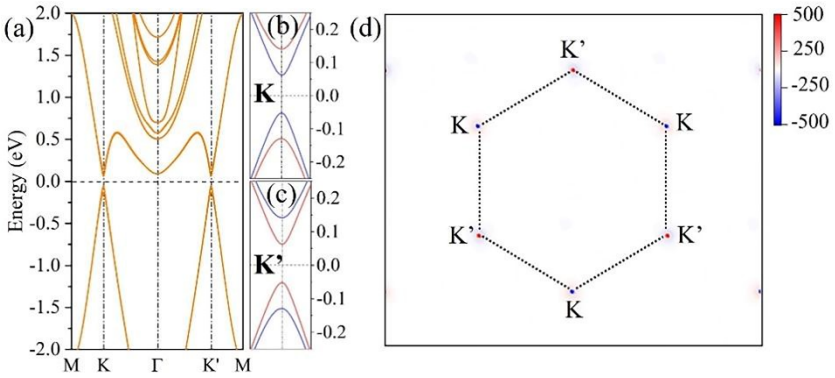

Fig. S5 (a) Calculated SOC band structures of the monolayer $AsCH_2OH$ with a 180° rotation. (b-c) The enlarged views of energy bands at K and K' valleys, respectively. The red and bule lines separately represent spin-up and spin-down states. (d) Calculated Berry curvatures in the Brillouin zone.

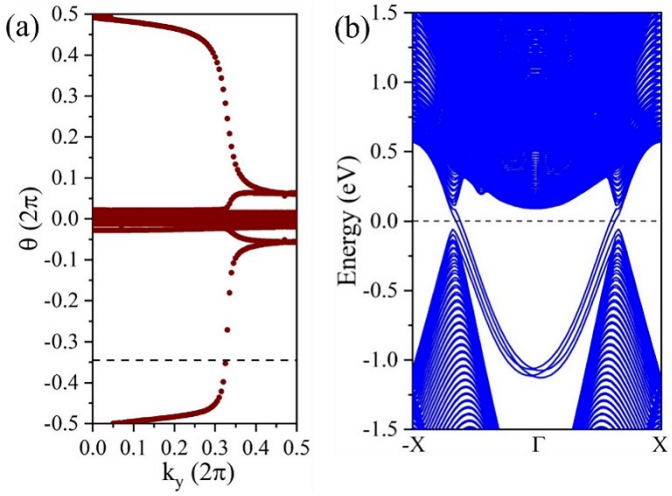

Fig. S6 Evolution of Wannier charge center and edge states for the monolayer $AsCH_2OH$ with a 180° rotation.