Supplementary Information (SI) for Physical Chemistry Chemical Physics.
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Supporting Information

Novel mixed topological state in monolayer $MnSbO_3$

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To evaluate the its stability, the phonon spectra, ab initio molecular dynamics (AIMD) simulation at 300 K and formation energy of monolayer $MnSbO_3$ are calculated. As shown in Figure S1(a), the absence of imaginary frequencies in the phonon spectra confirms the dynamical stability of the material. During the AIMD simulations, the total energy fluctuates within a small range, as demonstrated in Figure S1(b). Furthermore, the inset of Figure S1(b) shows that after 6 ps of AIMD simulations, the structure of monolayer $MnSbO_3$ remains intact, indicating its thermal stability. Furthermore, the formation energy of the monolayer $MnSbO_3$ is also studied, which is defined as $E_f = E_{total} - 2E_{Mn} - 2E_{Sb} - 6E_O$. Here, E_{total} is the ground state energy of monolayer $MnSbO_3$ in the primitive cell. E_{Mn}, E_{Sb} and E_O is the energy per atom of Mn, Sb and O in their most stable phases, respectively. The calculated values of E_f for monolayer $MnSbO_3$ is -15.69 eV (shown in Table S1), which is lower than that of monolayer $NiAsO_3$ (-10.62 eV) [1] and $MnAsO_3$ (-11.12 eV) [2], demonstrating that monolayer $MnSbO_3$ have a good thermodynamical stability against the elemental phases.

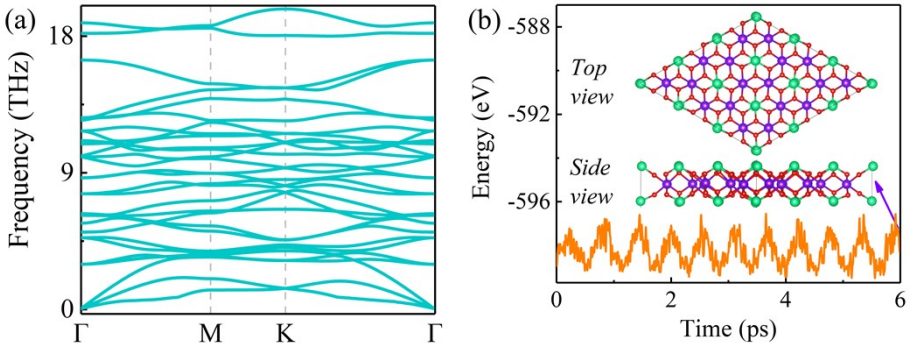

Figure S1. (a) Phonon spectrum of monolayer $MnSbO_3$. (b) Total energy fluctuation of the AIMD simulations for monolayer $MnSbO_3$. Inset is the structure of monolayer $MnSbO_3$ at 6 ps.

Table S1. The values of E_f, E_{total}, E_{Mn}, E_{Sb} and E_O for monolayer $MnSbO_3$.

Material	E_{total} (eV)	E_{Mn} (eV)	E_{Sb} (eV)	E_O (eV)	E_f (eV)
$MnSbO_3$	-22.39	-5.87	-4.15	-1.91	-15.69

Figure S2 displays one ferromagnetic (FM) and three antiferromagnetic (AFM1, AFM2 and AFM3) configurations of monolayer $MnSbO_3$.

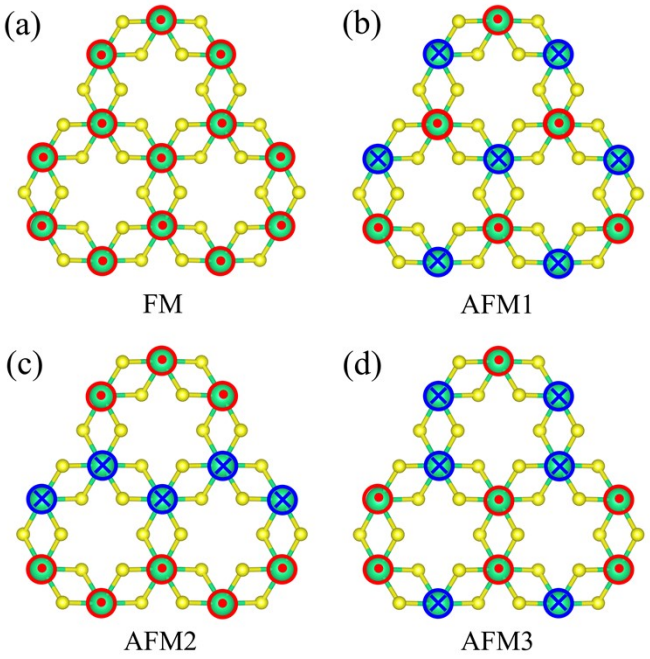

Figure S2. One ferromagnetic (FM) and three antiferromagnetic (AFM1, AFM2 and AFM3) configurations of monolayer $MnSbO_3$.

At φ = 5˚, 10˚, 15˚, 20˚ and 25˚ in xy plane, topological gap of monolayer $MnSbO_3$ decreases gradually, as shown in Figures S3(a)-S3(e). As φ = 90˚, monolayer $MnSbO_3$ presents a half metal state, as indicated in Figure S3(f). Under φ = 120˚ case, monolayer $MnSbO_3$ recovers the QAH states, as described in Figure S3(g). At φ = 150˚and 180˚, monolayer $MnSbO_3$ behaves as a half metal and QAH insulators, respectively, as shown in Figures S3(h) and S3(i).

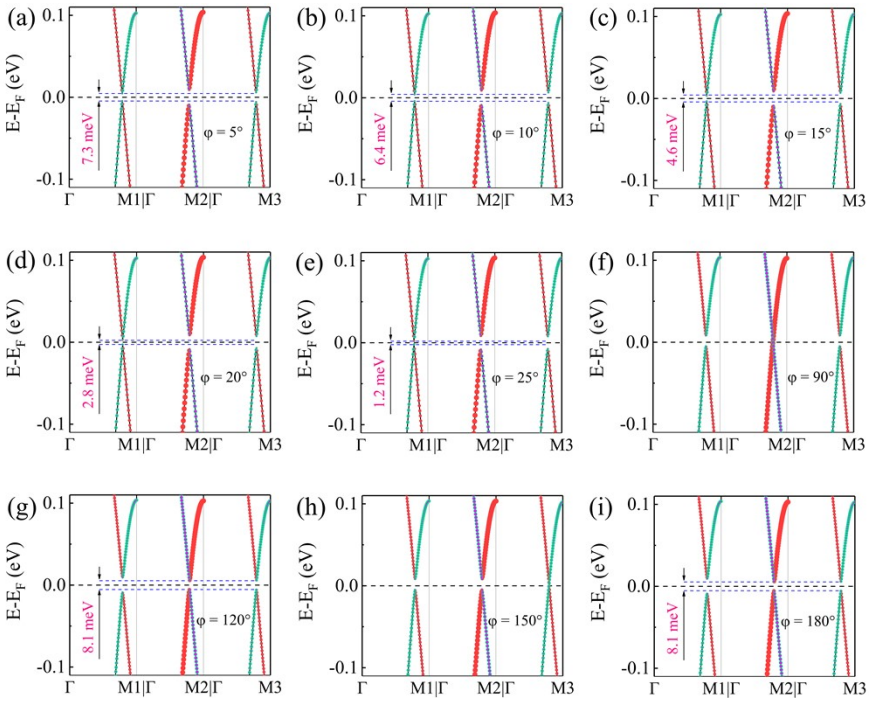

Figure S3. Orbital-resolved energy bands of monolayer $MnSbO_3$ as M direction varies in xy plane.

Figure S4 shows the orbital-resolved energy bands of monolayer $MnSbO_3$ as the M direction varies in xz plane. As θ changes from 30˚ to 180˚, the topological band gap of monolayer $MnSbO_3$ increases first, and then decreases, as shown in Figures S4(a)-S4(f).

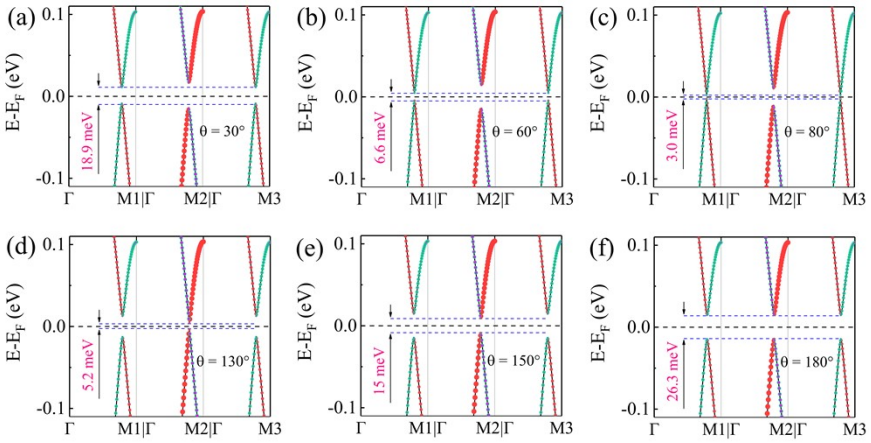

Figure S4. Orbital-resolved energy bands of monolayer $MnSbO_3$ as the M varies in xz plane.

As shown in Figure S5, under -5% ~ 5% strains, monolayer $MnSbO_3$ exhibits a QAH state as the M direction along φ = 0˚. Moreover, during this progress, the topological band gap of monolayer $MnSbO_3$ gradually decreases from 9.6 to 6.7 meV.

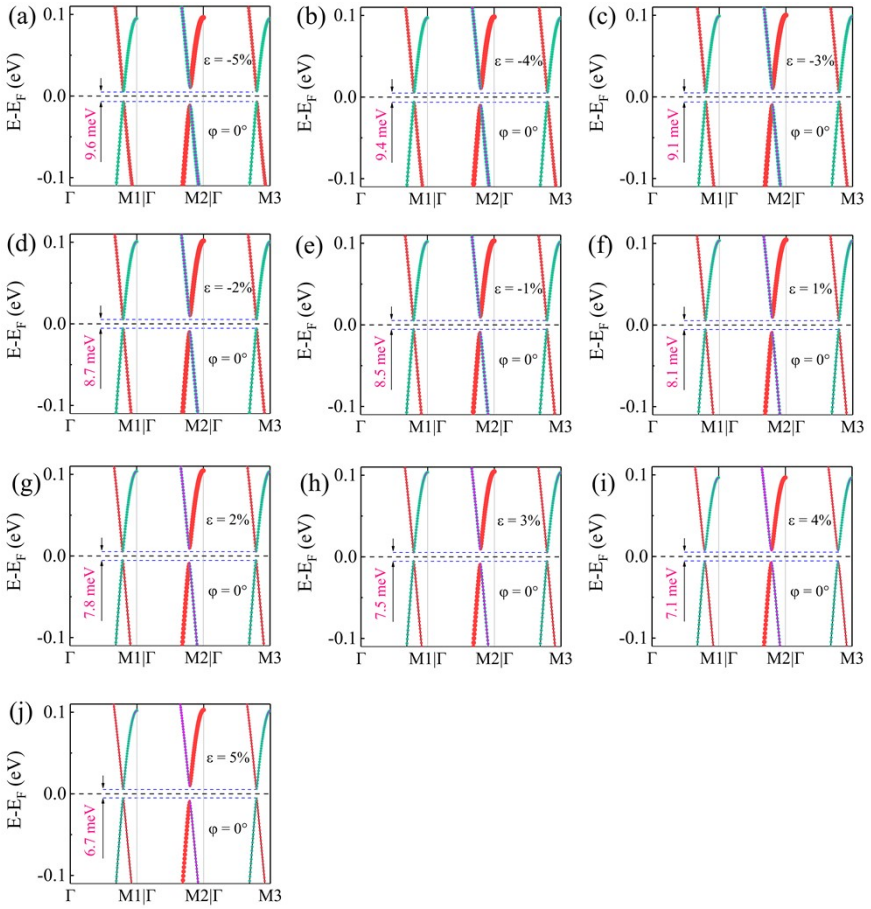

Figure S5. The orbital-resolved energy bands of monolayer $MnSbO_3$ under different strains as the M direction along φ = 0˚, respectively.

As drawn in Figures S6, under -5% ~ 5% strains, monolayer $MnSbO_3$ behaves as a QAH insulator as the M direction along θ = 0°. Moreover, throughout the strains, the topological band gap of monolayer $MnSbO_3$ also reduces from 26.9 to 24.9 meV.

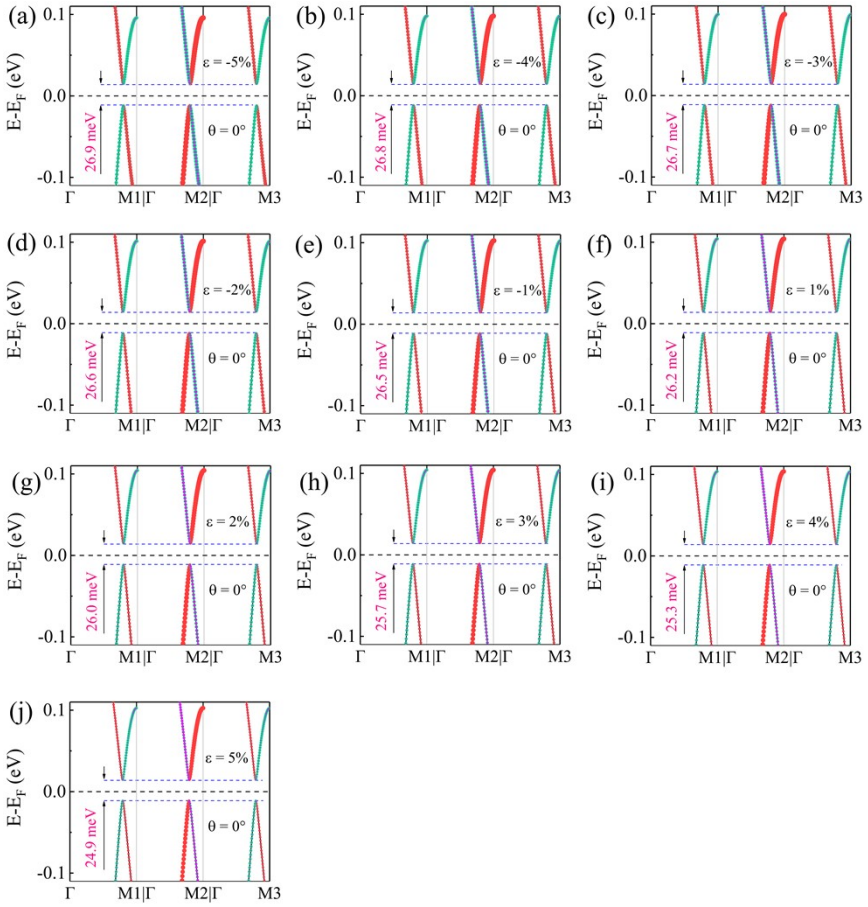

Figure S6. The orbital-resolved energy bands of monolayer $MnSbO_3$ under different strains as the M direction along θ = 0°, respectively.

As shown in Figures S7(a)-S7(f), under 0 ~ 5 eV U values, monolayer $MnSbO_3$ exhibits a QAH state as the M direction along φ = 0°. Moreover, during this progress, the topological band gap of monolayer $MnSbO_3$ gradually decreases from 9.2 to 7.9 meV. As drawn in Figures S7(g)-S7(l), under 0 ~ 5 eV U values, monolayer $MnSbO_3$ behaves as a QAH insulator as the M direction along θ = 0°. Moreover, throughout the strains, the topological band gap of monolayer $MnSbO_3$ also reduces from 38.3 to 24.2 meV. Therefore, the QAH property of monolayer $MnSbO_3$ is robust for strains and U values.

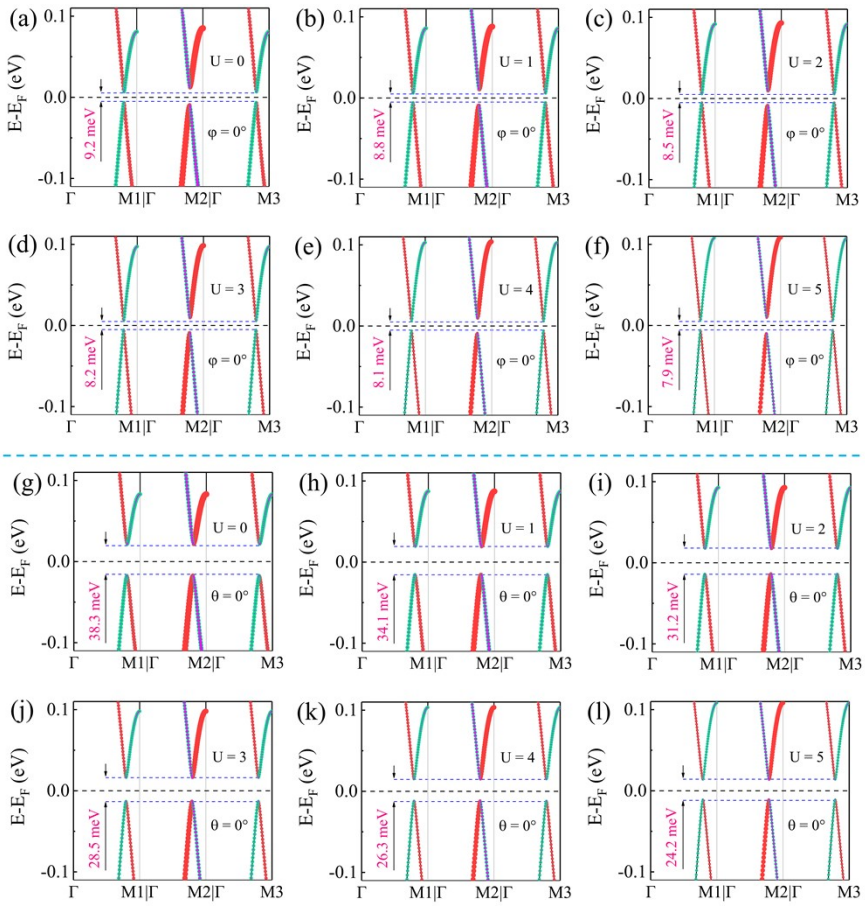

Figure S7. The orbital-resolved energy bands of monolayer $MnSbO_3$ under different U values as the M direction along φ = 0˚ and θ = 0˚, respectively.

References

[1] Z. Y. Li, Y. L. Han, Z. H. Qiao. Chern number tunable quantum anomalous Hall effect in monolayer transitional metal oxides via manipulating magnetization orientation. *Phys. Rev. Lett.* **129**, 036801 (2022).

[2] H. Chen, J.n Lu, N. Wang, X. Zhao, G. Hu, X. Yuan, and J. Ren, Strain-induced high-Chern-number spin-unlocked edge states in monolayer $MnAsO_3$ with intrinsic quantum anomalous Hall effect, *Appl. Phys. Lett.* **124**, 153101 (2024).