Supplementary Information (SI) for Journal of Materials Chemistry C.
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Quantum anomalous Hall effect in novel two-dimensional structure Ta_2Se_3

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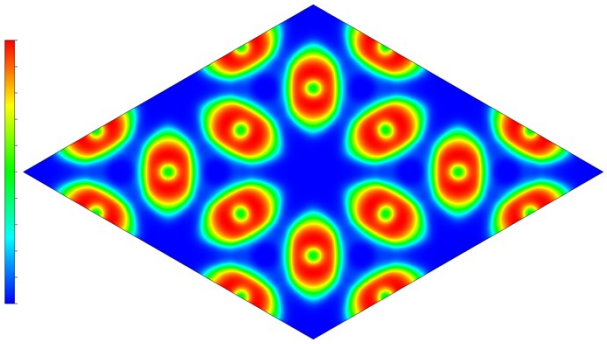

Fig. S1 The electron localization function of the Ta_2Se_3 ML is clearly characterized by ionic bonding between Ta and Se atoms, where red denotes electron localization and blue denotes electron delocalization.

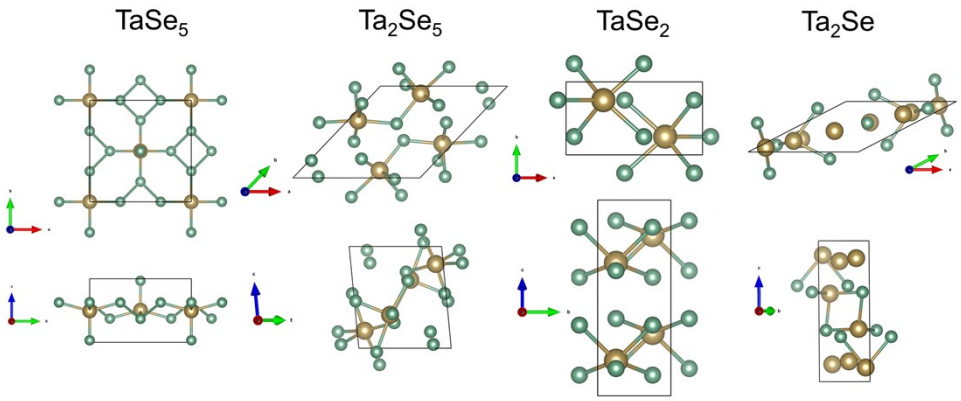

Fig.S2 Top and side views of the 3D structures composed of Ta and Se elements in the convex hull diagram.

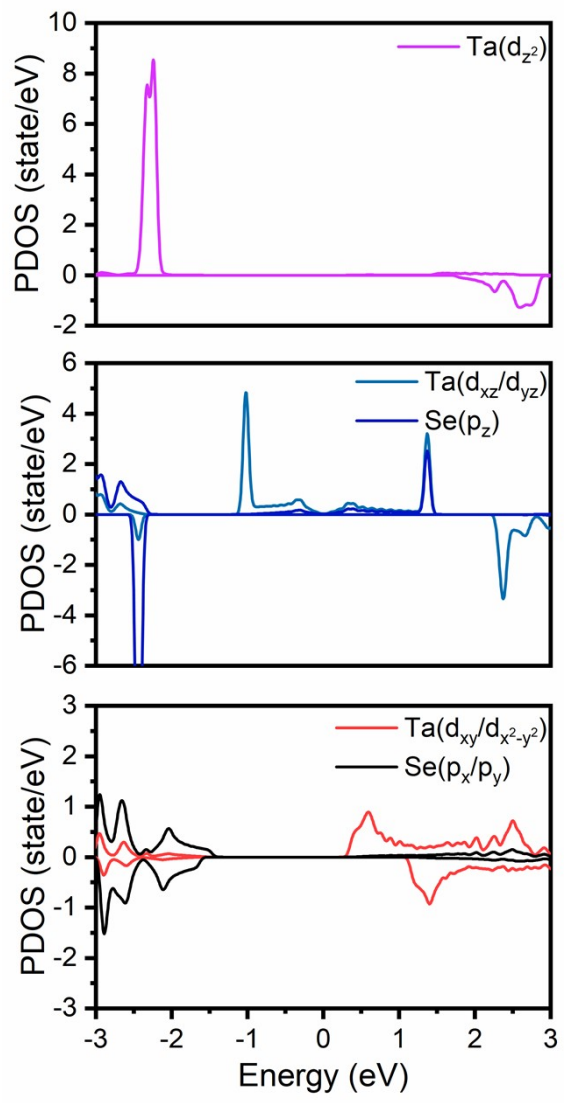

Fig. S3 Orbital decomposition density of states (DOS) plot.

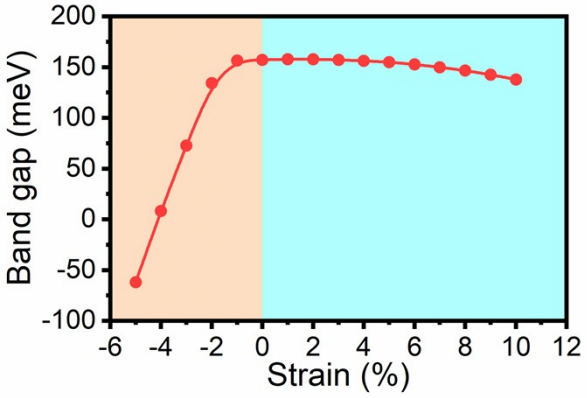

Fig. S4 The effect of strain on band gap, with negative strain representing compression and positive strain representing tension.

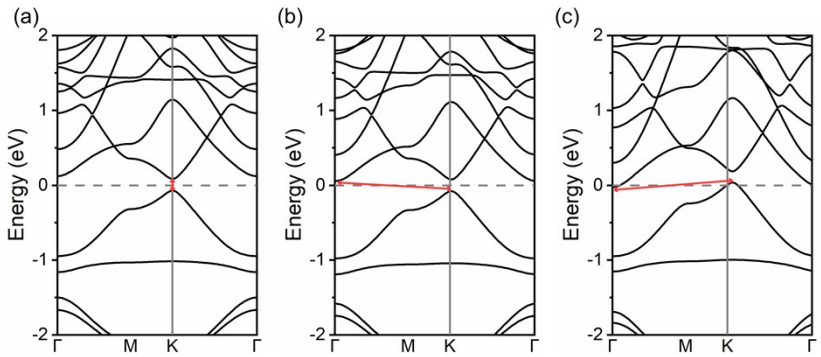

Fig. S5 Band structure with SOC under different cases of strain (a)-1% (b)-2% (c)-5%. At -1% compressive strain, it exhibits a direct bandgap; at -2% compressive strain, it is an indirect bandgap; and at -5% compressive strain, it not only exhibits an indirect bandgap but also a metallic bandgap.

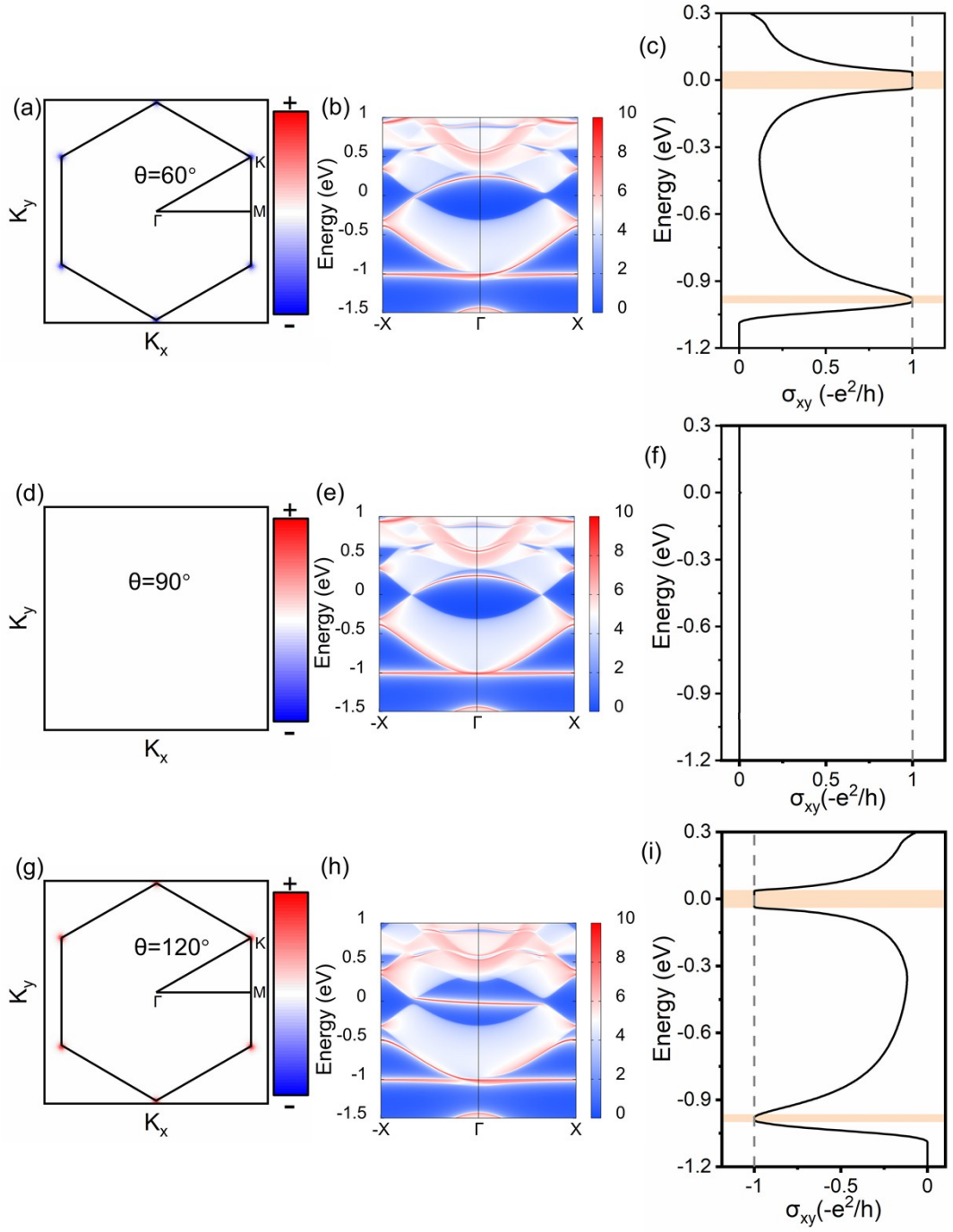

Fig. S6 Topological properties in various spin directions. (a-c) Topological correlation properties at θ = 60°, which are similar to those with θ = 0° because the spin orientation has a component in the +z axis. (d-f) Topological correlation properties with θ = 90°, the system is in a trivial state, so the net Berry curvature is zero, the anomalous Hall conductivity vanishes, and there are no chiral edge states. (g-i) The properties at θ = 120° are similar to those at θ = 60° due to the spin orientation having a component in

the -z axis, but the Berry curvature and anomalous Hall conductivity have opposite signs.

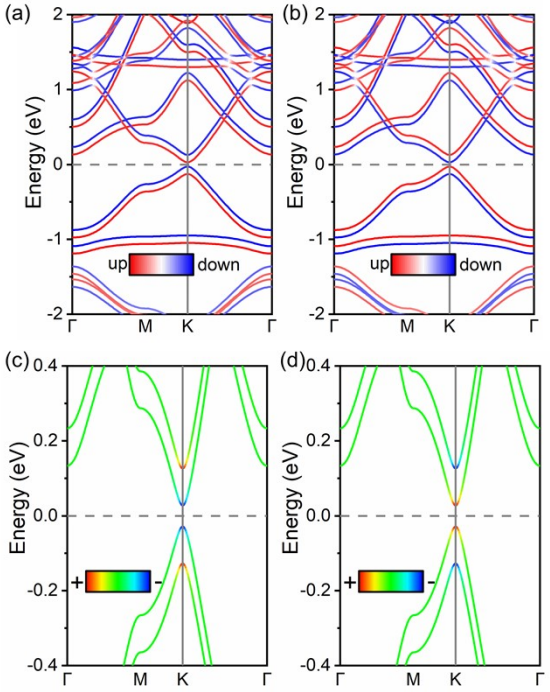

Fig. S7 (a-b) Spin projections of Ta_2Se_3 B under (a) 0.2 V/nm and (b) -0.2 V/nm electric fields, where red and blue colors denote spin-up and spin-down projections in the z direction, respectively. (c-d) Berry curvature projections of Ta_2Se_3 BL under (c) 0.2 V/nm and (d) -0.2 V/nm electric fields, where red represents positive values and blue represents negative values.