Supplementary Information

Tuning the magnetic state and topological transition of monolayer Kagome Co_3Pb_3SSe with large magnetic Anisotropy

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The contribution of the orbit affects the magnetic anisotropy through spin-orbit coupling, the MAE having the same spin coupling upward (uu) or downward (dd) is expressed as

$$MAE_{uu/dd} = E_z - E_x = \xi^2 \sum_{ou} \frac{|\langle o|L_x|u\rangle|^2 - |\langle o|L_z|u\rangle|^2}{E_u - E_o} \quad \text{(S1)}$$

where $\langle o|$ ($\langle u|$) donates the occupied(unoccupied) states, ξ^2 represents the spin-orbit coupling constant.L_x and L_z are the x-component and z-component of angular momentum operators. When having opposite spin (ud) coupling, the MAE is expressed as

$$MAE_{ud} = E_z - E_x = \xi^2 \sum_{ou} \frac{|\langle o|L_z|u\rangle|^2 - |\langle o|L_x|u\rangle|^2}{E_u - E_o} \quad \text{(S2)}$$

The orbital angular momentum with d_{z2} ,d_{xy} , d_{x2-y2} , d_{xz} ,d_{yz} and p_x , p_y ,p_z as the basis group are respectively expressed as

$$L_z = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 2i & 0 & 0 \\ 0 & -2i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & -i \\ 0 & 0 & 0 & i & 0 \end{bmatrix} \quad L_x = \begin{bmatrix} 0 & 0 & 0 & 0 & \sqrt{3}i \\ 0 & 0 & -i & 0 & 0 \\ 0 & 0 & 0 & i & 0 \\ 0 & i & 0 & 0 & 0 \\ -\sqrt{3}i & 0 & -i & 0 & 0 \end{bmatrix}$$

$$L_z = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -2i \\ 0 & 2i & 0 \end{bmatrix} \quad L_x = \begin{bmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \quad \text{(S3)}$$

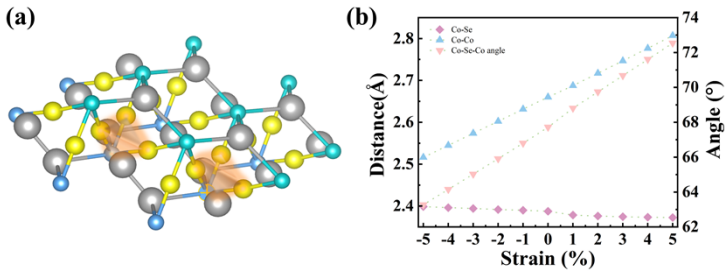

Fig. S1. (a) the monolayer Co_3Pb_3SSe structure considering magnetic interactions, with yellow representing three Co atoms forming a triangle; bond length and bond Angle as functions of applied biaxial strain.

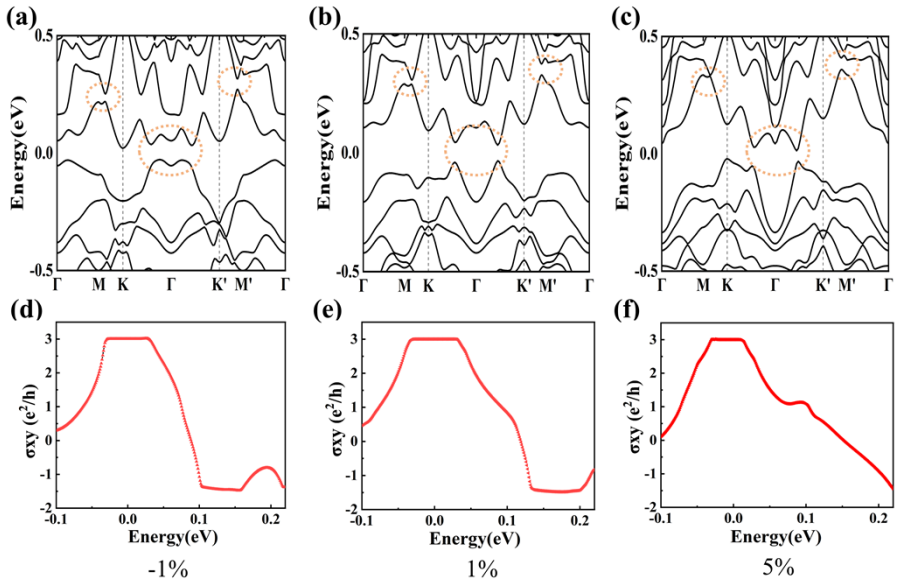

Fig. S2. Energy band structures with SOC of Co_3Pb_3SSe monolayer under different strains.(a)-1%, (b)1%, (c)5%. (d)-(f) The corresponding anomalous Hall conductance,respectively.

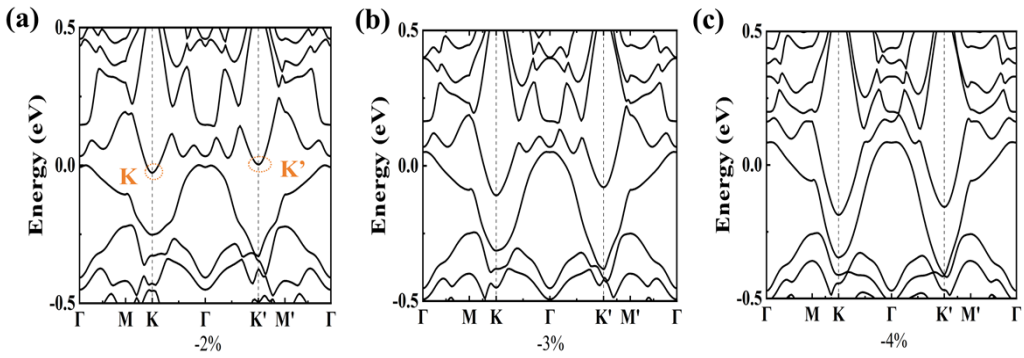

Fig. S3. Energy band structures with SOC of Co_3Pb_3SSe monolayer under different strains.(a)-2%, (b)-3%, (c)-4%. All are metallic state.