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

Supplemental Material

Electric field and strain engineering tuning Rashba spin splitting in quasi-one-dimensional organic-inorganic hybrid perovskites (MV)AI$_3$Cl$_2$ (MV = methylviologen, A = Bi, Sb)

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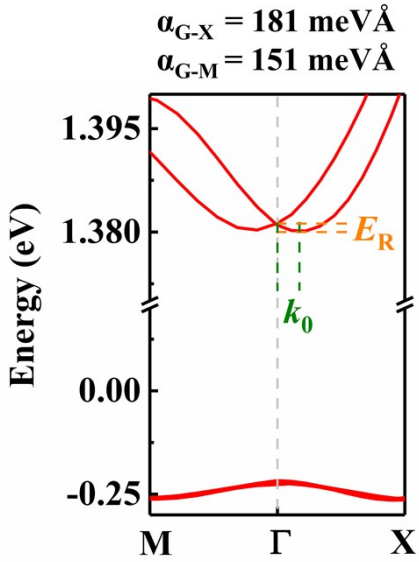

Fig. S1. The band structure of k_x–k_y plane (MV)BiI_3Cl_2 with different Rashba constants were calculated using HSE06 hybrid functionals.

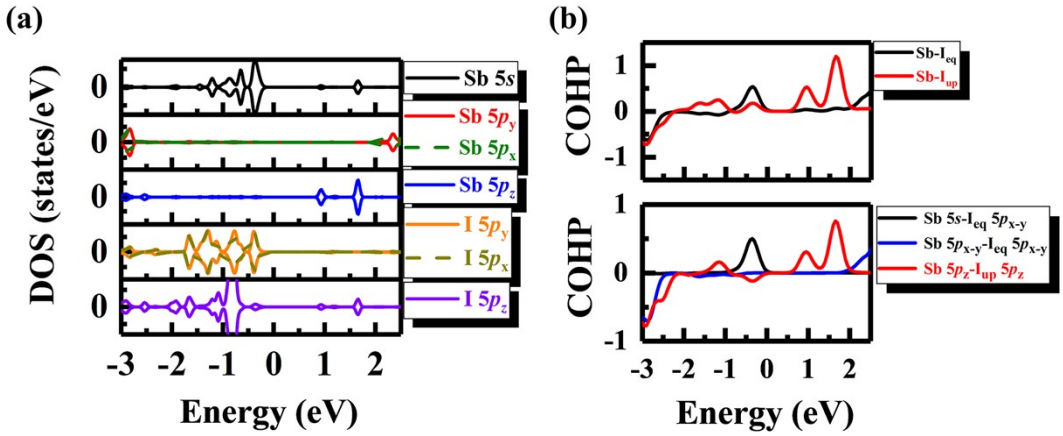

Fig. S2. (a) The projected denisty of states (DOS) of Sb and I atoms in (MV)SbI_3Cl_2. (b) The Crystal Orbital Hamilton Population (COHP) of Sb and its neighboring I atoms.

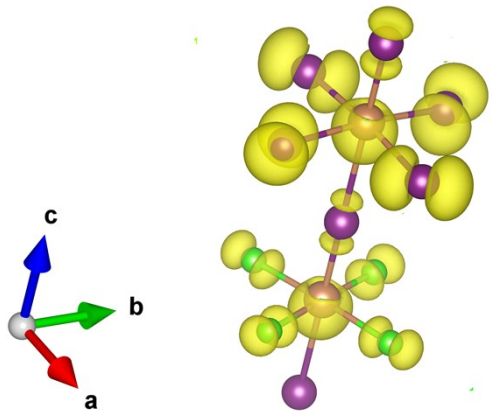

Fig. S3. (a) The partial charge density of the valence band maximum of $(MV)SbI_3Cl_2$.

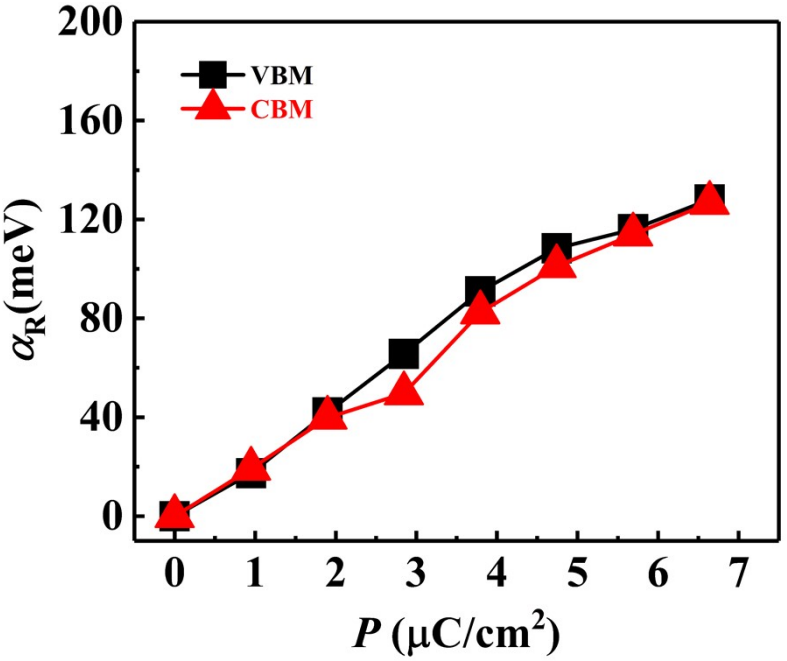

Fig. S4. The Rashba constant of the VBM and the CBM for $(MV)SbI_3Cl_2$ with polarization.