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Hot carrier relaxation in $Cs_2TiI_yBr_{6-y}$ (y = 0, 2 or 6) by time-domain ab initio study

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The fluctuation of band edge of $Cs_2TiI_yBr_{6-y}$ in 5ps adiabatic MD process are listed in Fig. S1. Hot carrier relaxation are intraband band processes. The carriers in higher energy state relax toward the band edge with the relaxation rate determined by the NAC values inner CB or VB region. The fluctuation of band edge should not affect the relaxation of hot carrier significantly.

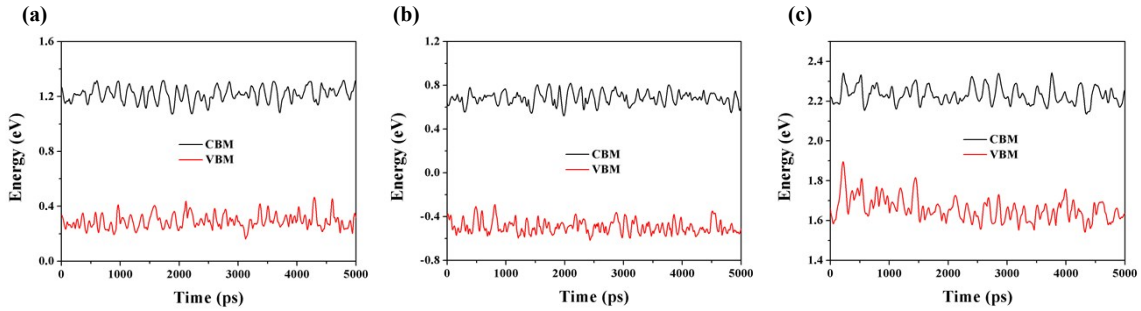

Fig. S1. The fluctuation of band edge for $Cs_2TiI_yBr_{6-y}$ in 5ps adiabatic MD process. a) fluctuation of CBM and VBM in Cs_2TiBr_6; b) fluctuation of CBM and VBM in $Cs_2TiI_2Br_4$; c) fluctuation of CBM and VBM in Cs_2TiI_6.

As shown in Fig. S2, the CBM of $Cs_2TiI_yBr_{6-y}$ arise from the Ti-3d orbitals and the VBM arise from the p orbitals of halogen. With this scenario, different electrons and holes localization are formed.

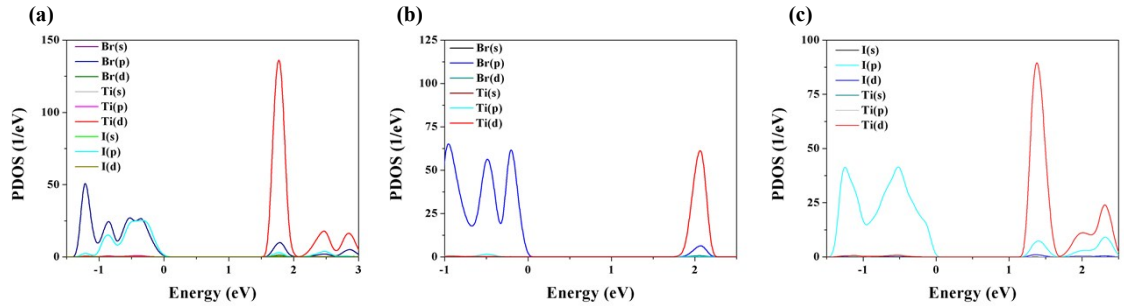

Fig. S2. The orbital split PDOS of $Cs_2TiI_yBr_{6-y}$. a) orbital split PDOS diagram of Cs_2TiBr_6; b) orbital split PDOS diagram of $Cs_2TiI_2Br_4$; c) orbital split PDOS diagram of Cs_2TiI_6.