Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.
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Supporting Information

Structure modulation for bandgap engineered vacancy-ordered $Cs_3Bi_2Br_9$ perovskite structures through copper alloying

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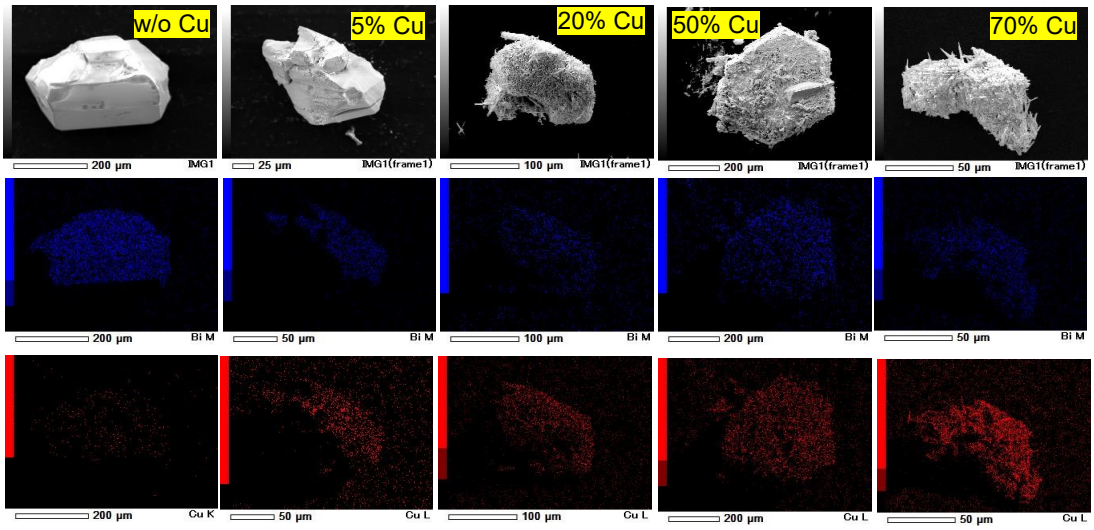

Fig. S1 Scanning Electron Microscope (SEM) images of perovskite crystals with different Cu-alloying with Energy Dispersive Scanning (EDS) elemental mapping for Bi (Blue) and Cu (Red).

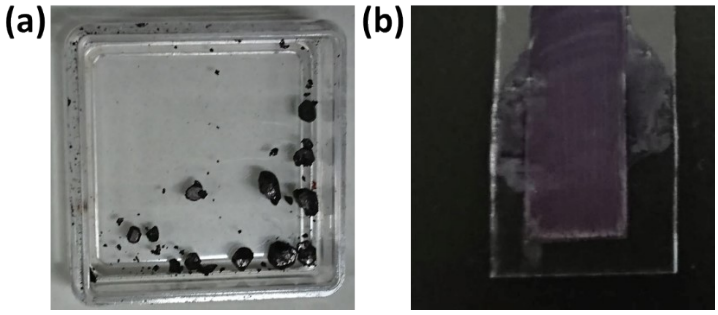

Fig. S2 (a) Photograph of Cs_2CuBr_4 perovskite crystals. (b) Photograph of drop-casted Cs_2CuBr_4 perovskite thin film over TiO_2/Glass substrate.

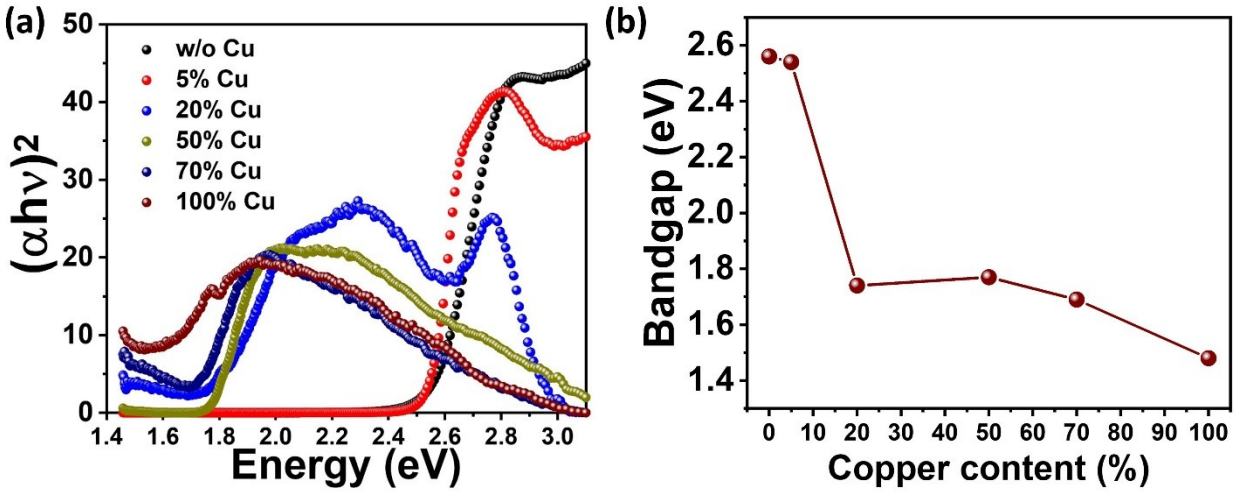

Fig. S3 Direct bandgap estimation: (a) Tauc plots of different Cu-alloyed perovskite thin films. (b) Bandgap energies of different Cu-alloyed perovskite thin films.

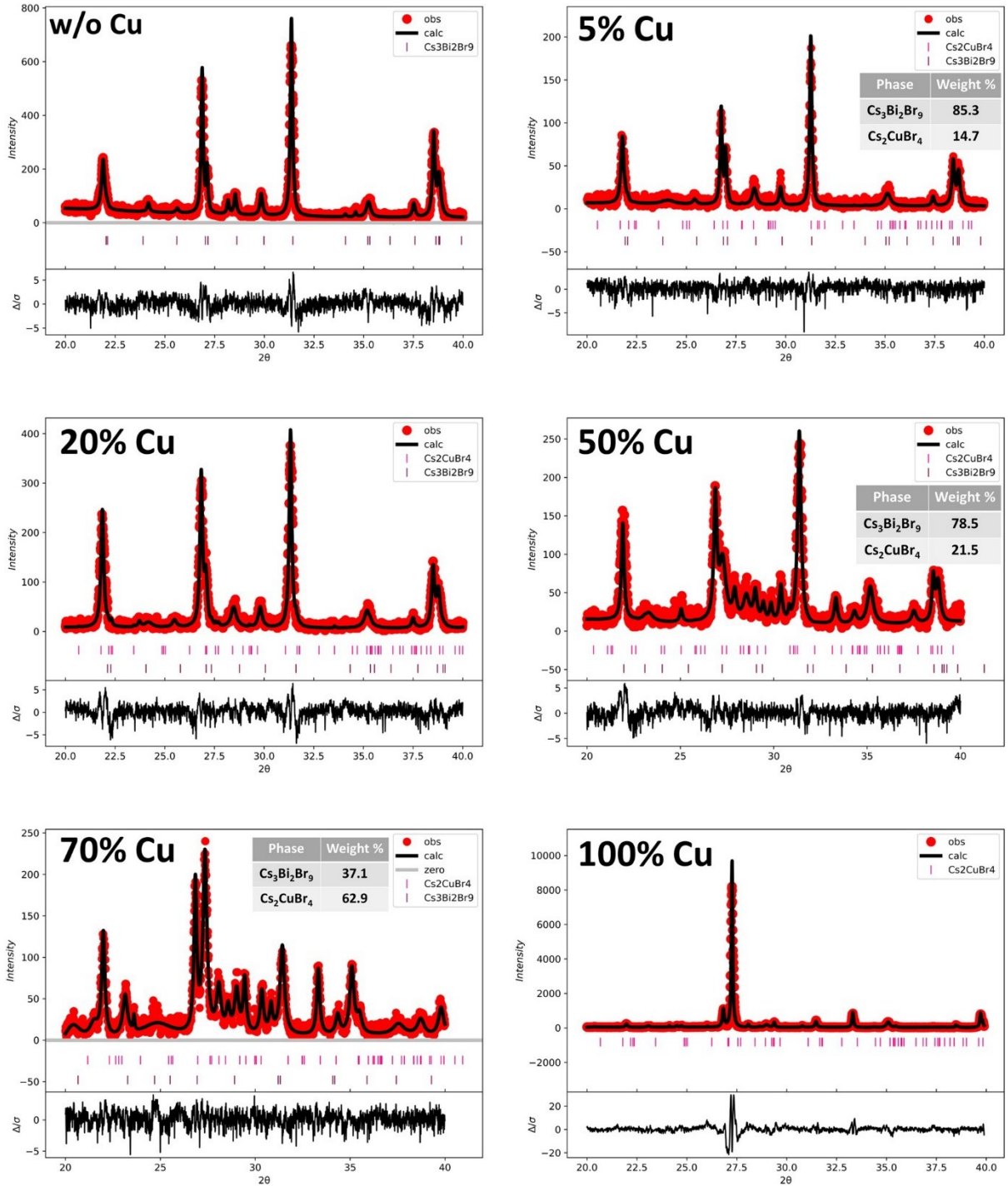

Fig. S4 Rietveld refinement spectra of different Cu-alloyed perovskite thin films.

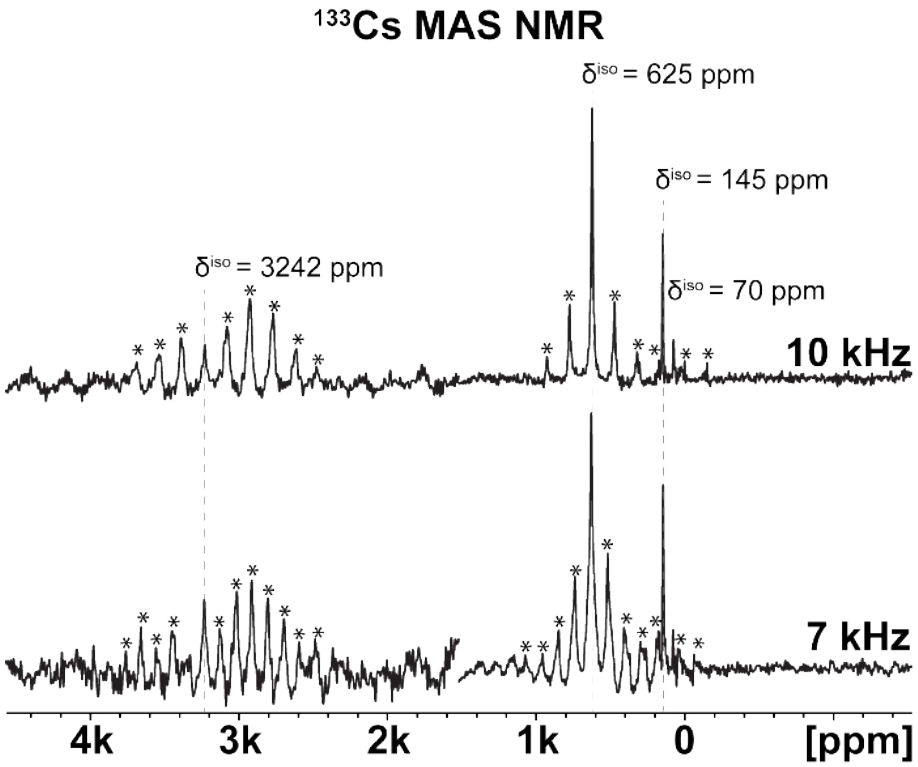

Fig. S5 Experimental 133Cs MAS NMR spectra of 70% Cu-alloyed perovskite were conducted at 10 kHz and 7 kHz spinning speeds of the sample. The asterisks (*) denote spinning sidebands.

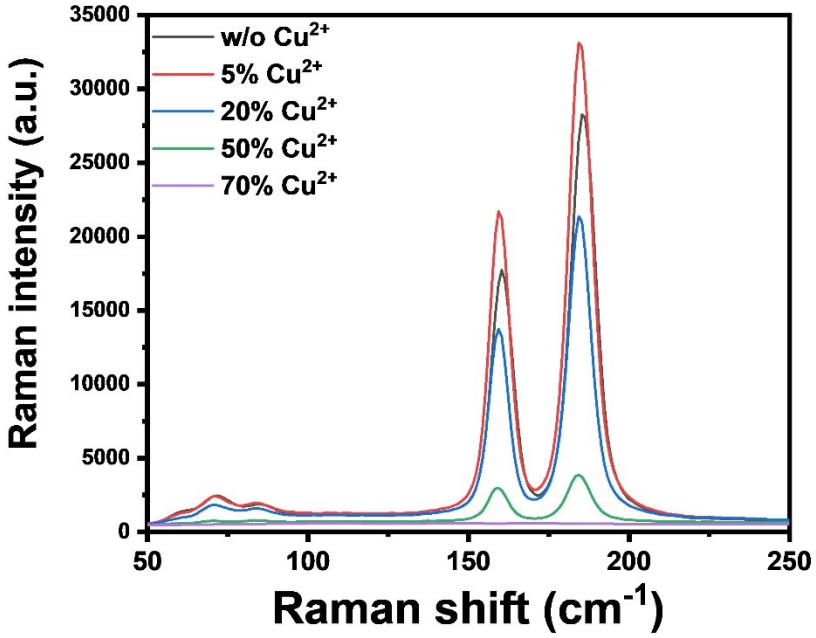

Fig. S6 Raman measurement of different Cu-alloyed perovskite crystals.

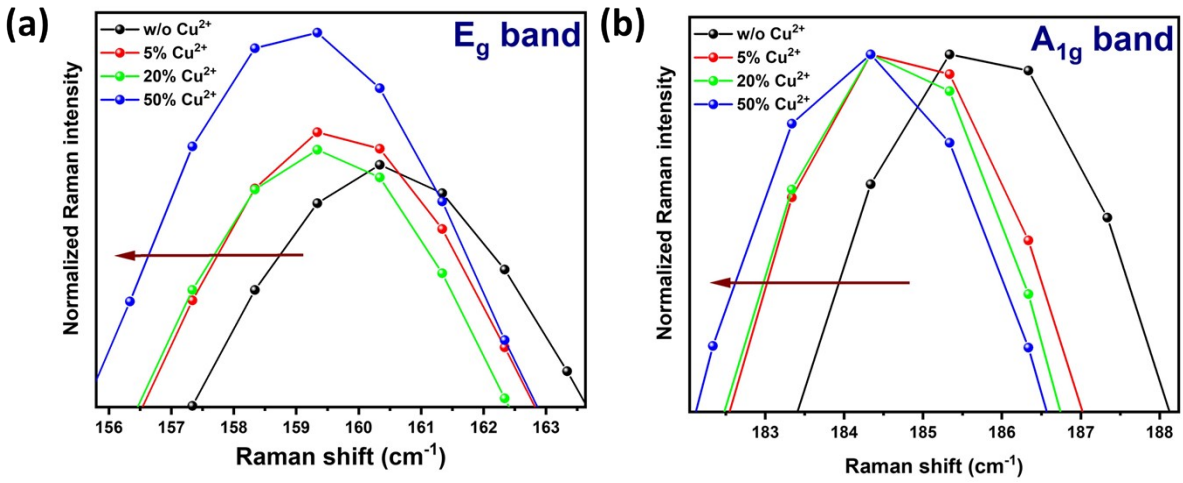

Fig. S7 Normalized Raman Eg (a), and A1g (b) bands for different alloyed Cu-$Cs_3Bi_2Br_9$ perovskites.

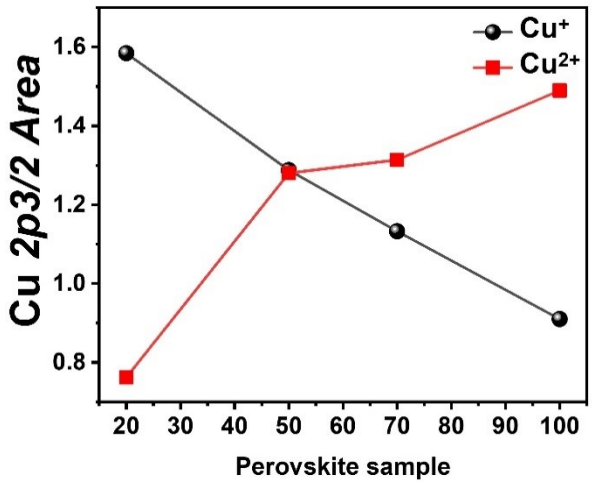

Fig. S8 XPS Cu $2p_{3/2}$ peak area of Cu^{2+} (Red square) and Cu^{+} (Black balls) for different alloyed Cu-$Cs_3Bi_2Br_9$ perovskites.

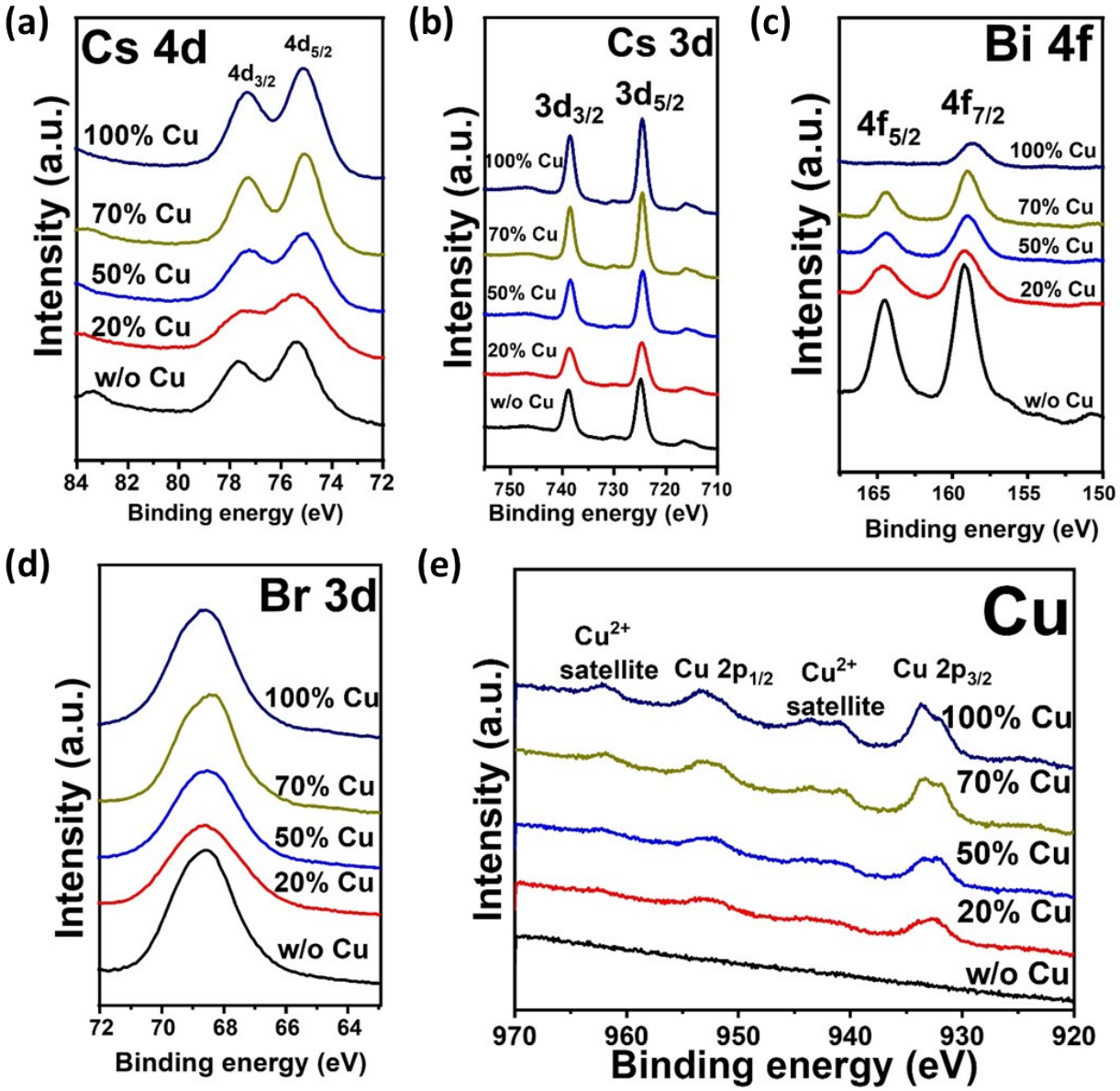

Fig. S9 XPS spectra of Cs 4d (a), Cs 3d (b), Bi 4f (c), Br 3d (d), and Cu 2p (e) for different alloyed Cu-$Cs_3Bi_2Br_9$ perovskites.

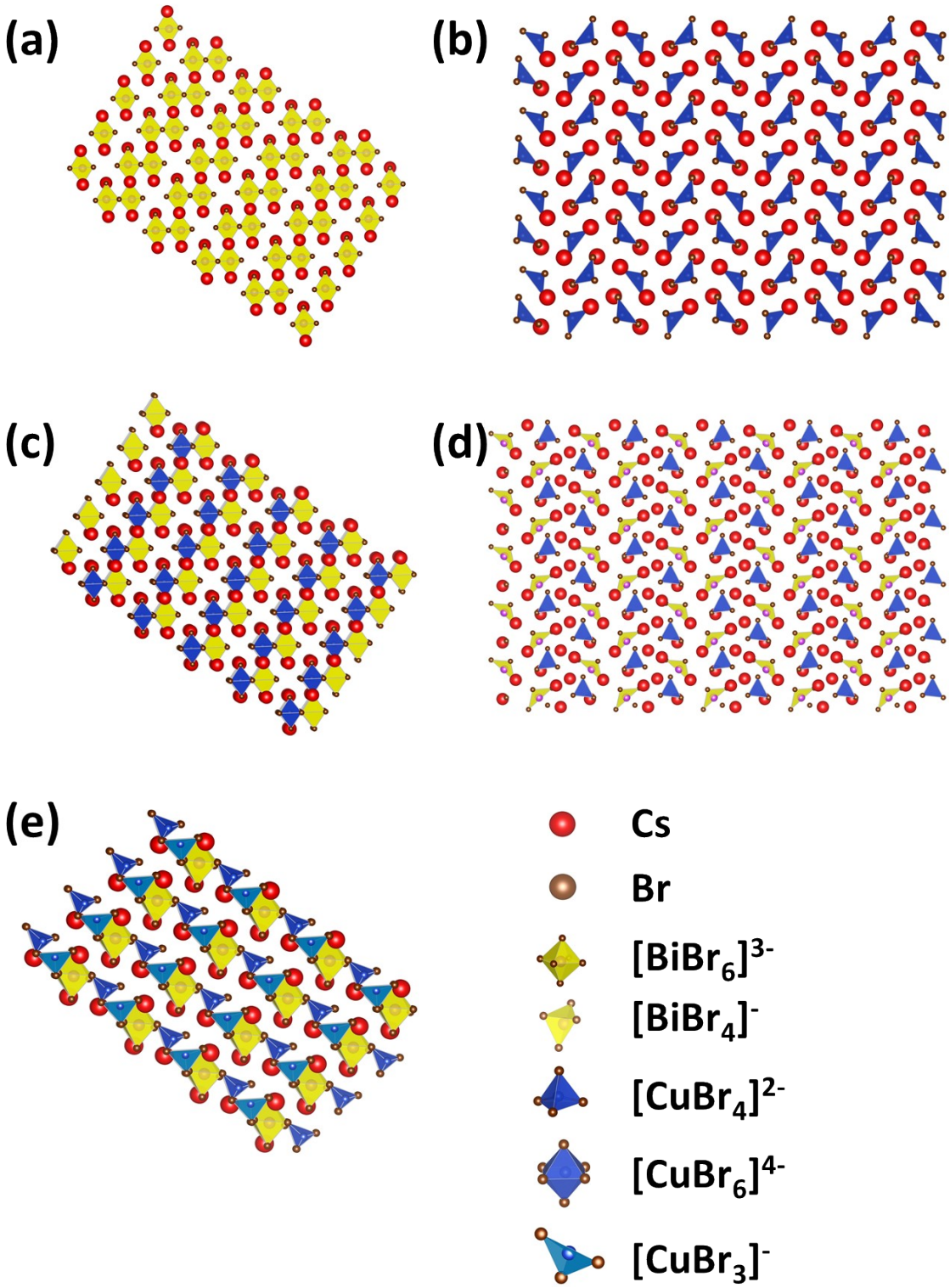

Fig. S10 Different perovskite crystal structures applied for calculating energy above the convex hull: (a) $Cs_3Bi_2Br_9$ (b) Cs_2CuBr_4 (c) 50%Cu-$Cs_3Bi_2Br_9$ (d) 50%Cu- Cs_2CuBr_4 (e) Cu_ $Cs_3Bi_2Br_9$ Cu_{Br} compensating defect.