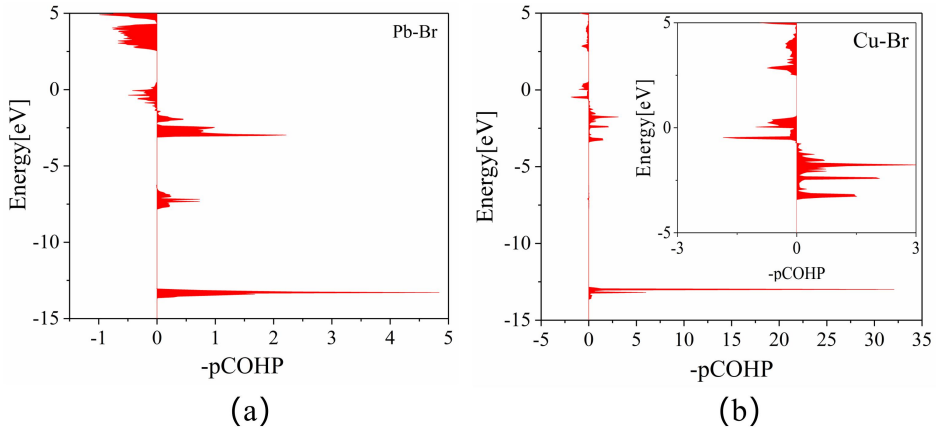


Figure S1. COHP analyses for (a) Pb-Br bond in [PbX_6] octahedron of pristine cubic $CsPbBr_3$, (b) Cu-Br bond in [CuX_6] octahedron of cubic $CsPb_{0.875}Cu_{0.125}Br_3$. The inset in (b) represents the COHP analyses with the energy from -5 eV to 5 eV for Cu-Br bond in $CsPb_{0.875}Cu_{0.125}Br_3$.

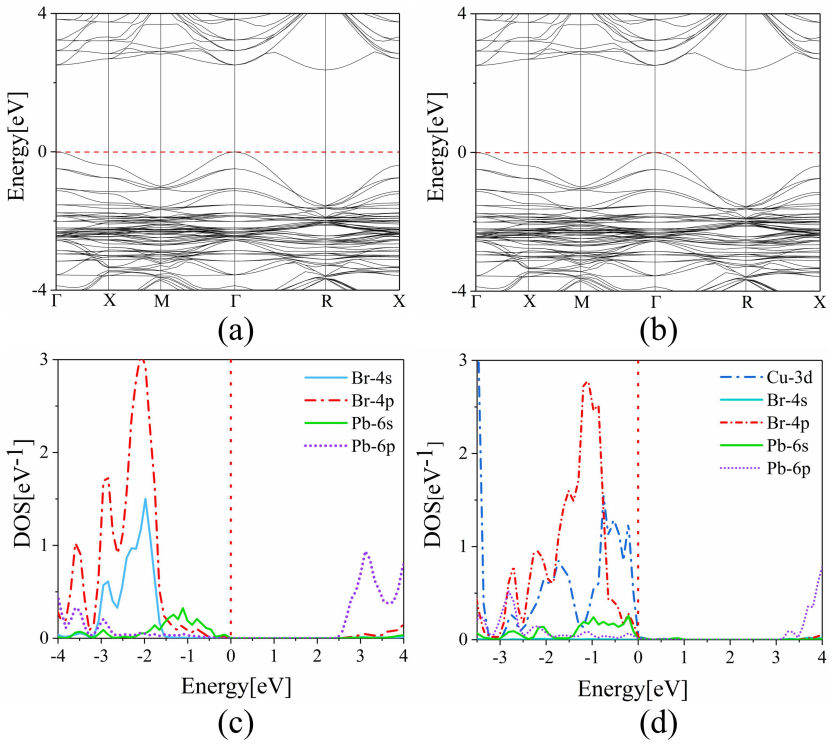


Figure S2. The band structures of cubic (a) $CsPbBr_3$ and (b) $CsPb_{0.875}Cu_{0.125}Br_3$ systems, respectively. The Partial density of states of cubic (c) $CsPbBr_3$ and (d) $CsPb_{0.875}Cu_{0.125}Br_3$ systems, respectively. All results are calculated via HSE functions.

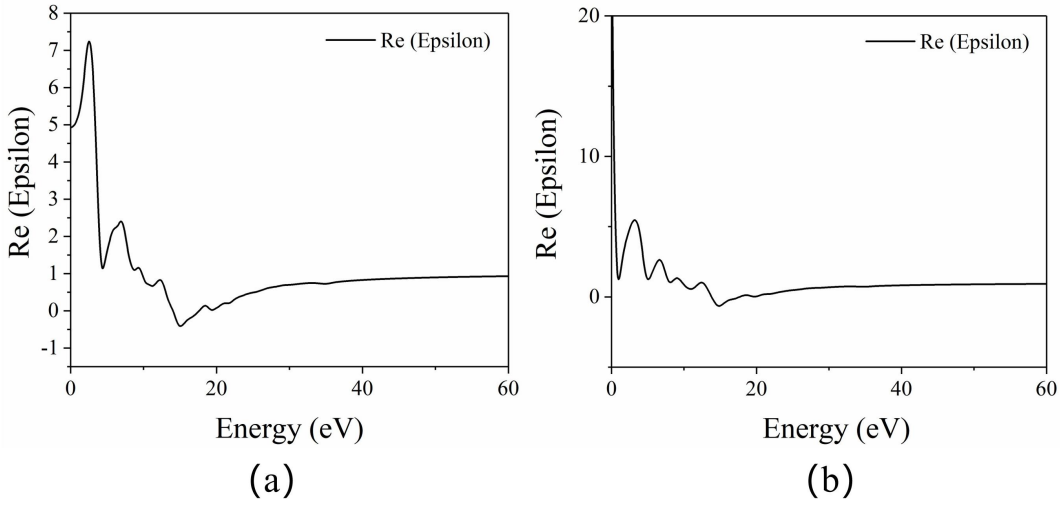


Figure S3. The refractive index of (a) $CsPbBr_3$ and (b) $CsPb_{0.875}Cu_{0.125}Br_3$ systems.