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

Electronic Supplementary Information

In- and Ga-based Inorganic Double Perovskites with Direct Bandgaps for Photovoltaic Applications

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The key parameters used for the HSE06 computation are: HFSCREEN = 0.2 (the range-separation parameter in range separated hybrid functionals), AEXX=0.25 (the fraction of exact exchange in a Hartree-Fock/DFT hybrid functional type calculation), and AGGAX=0.75 (the fraction of gradient corrections to the exchange in a Hartree-Fock/DFT hybrid functional type calculation).

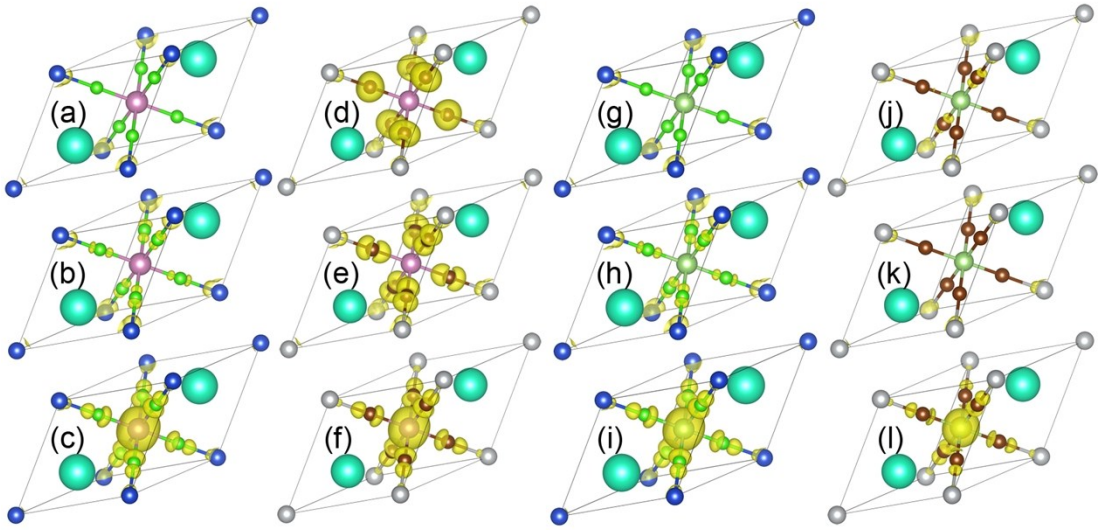

Figure S1. Iso-surface plot of the band-decomposed charge density of (a-c) $Cs_2CuInCl_6$, $Cs_2AgInBr_6$ (d-f), $Cs_2CuGaCl_6$ (g-i) and $Cs_2AgGaBr_6$(j-l); in each column, from top to down is the light hole band, heavy hole band and the lowest conduction band.