Electronic Supporting Information

Two-dimensional Optical Excitations in Mixed-Valence Cs$_2$Au$_2$I$_6$ Fully Inorganic Double Perovskite

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Fig. S1: (top) Cs$_2$Au$_2$I$_6$ DFT/PBE calculated Total Density of States and Projected Density of States on Au and I Orbitals; (bottom) Cs$_2$Au$_2$I$_6$ GW calculated bandstructure (with SOC: red line; without SOC: blue dashed line)
Fig. S2: Cs$_2$Au$_2$I$_6$ wavefunction square modulus (orange) of (a) Intermediate Band, (b) Intermediate Band [Mauve atoms: I, Blue atoms: Au; cyan atoms: Cs. isosurface 0.005 eV/Å]
Fig. S3: Top view of the wavefunction square modulus of the (a) first optically inactive (dark) and (b) first bright exciton. [Mauve atoms: I, Blue atoms: Au; cyan atoms: Cs. Orange isosurface represents the probability of finding the electron when the hole position (yellow spot) is fixed near a given atomic site.]