

Electronic Supporting Information

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

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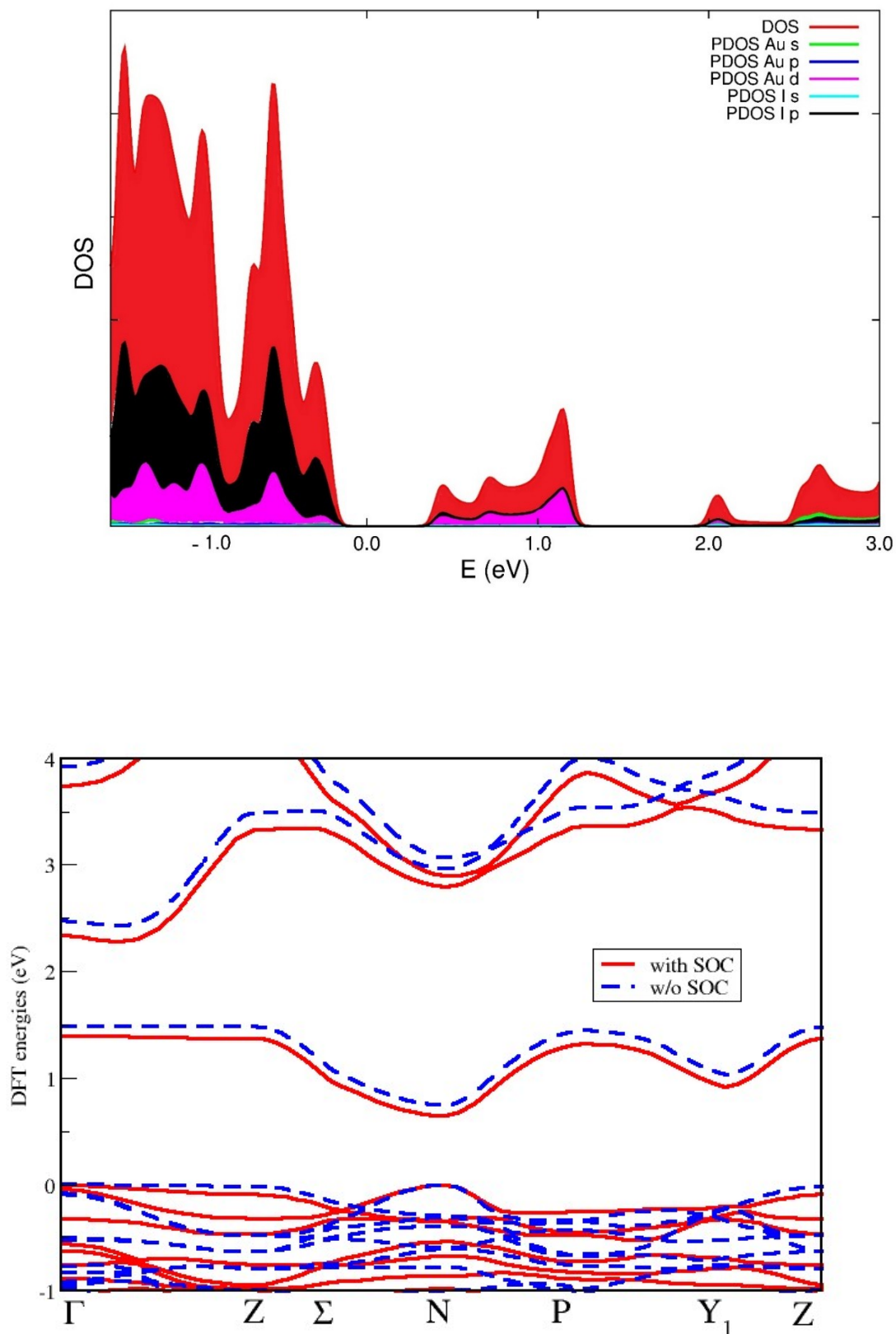


Fig.

S1: (top) $\text{Cs}_2\text{Au}_2\text{I}_6$ DFT/PBE calculated Total Density of States and Projected Density of States on Au and I Orbitals; (bottom) $\text{Cs}_2\text{Au}_2\text{I}_6$ GW calculated bandstructure (with SOC: red line; without SOC: blue dashed line)

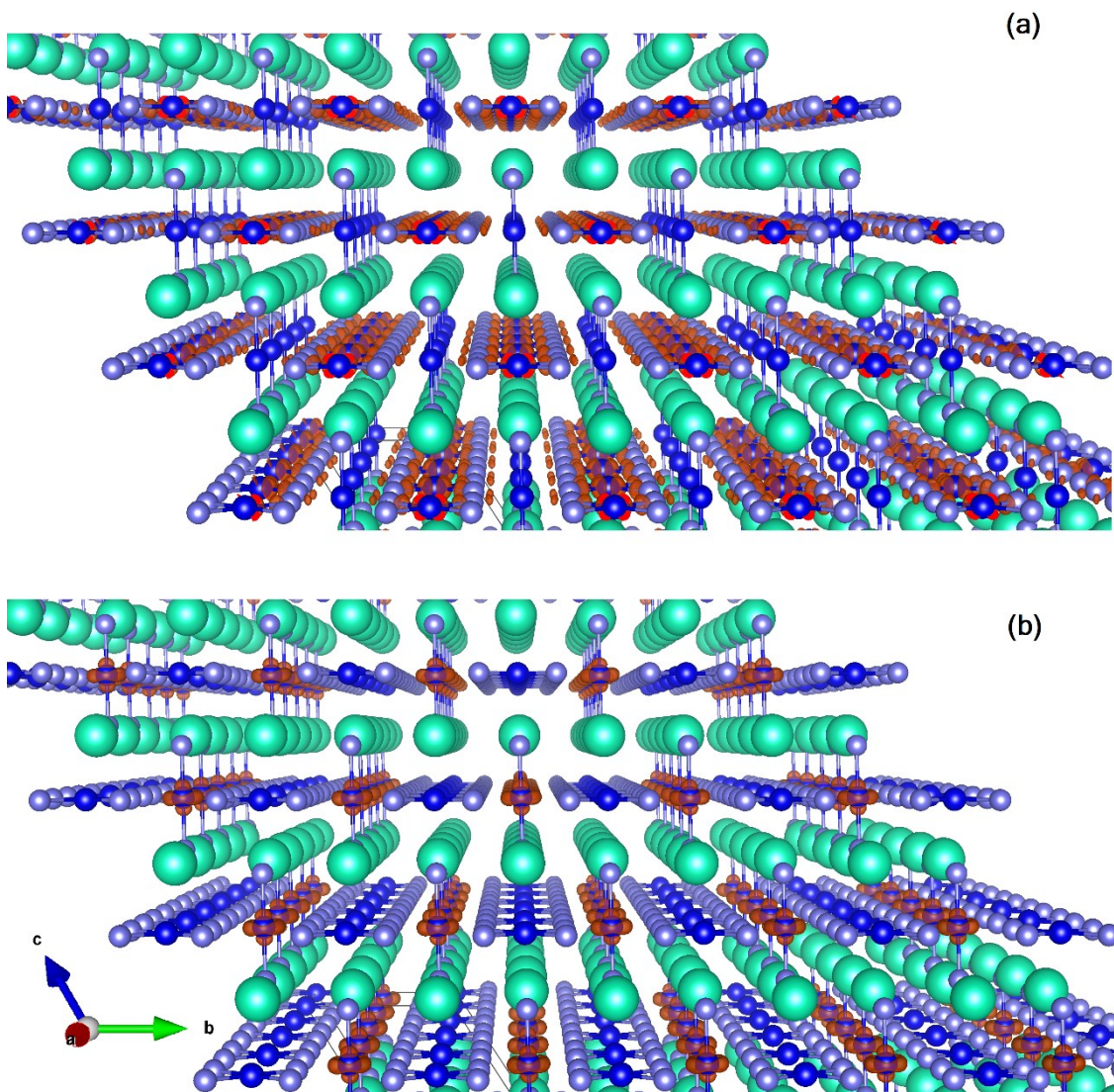
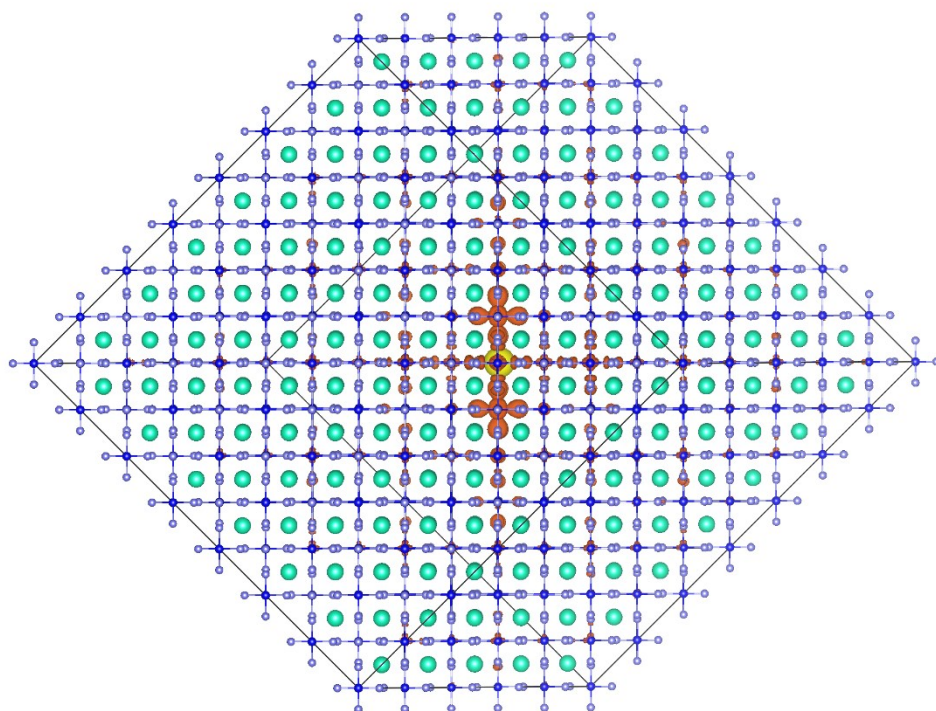


Fig. S2: $\text{Cs}_2\text{Au}_2\text{I}_6$ wavefunction square modulus (orange) of (a) Intermediate Band, (b) Intermediate Band [Mauve atoms: I, Blue atoms: Au; cyan atoms: Cs. isosurface $0.005 \text{ eV/\AA}$]

(a)



(b)

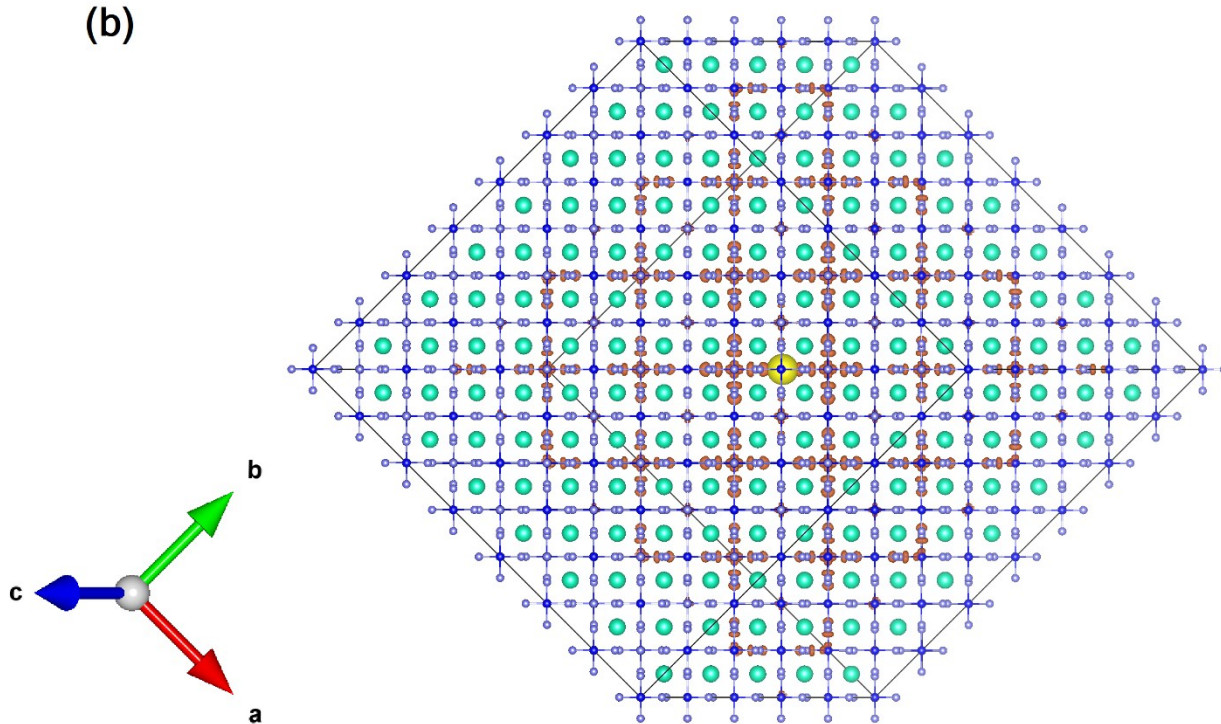


Fig. S3: Top view of the wavefunction square modulus of the (a) first optically inactive (dark) and (b) first bright exciton. [Mauve atoms: I, Blue atoms: Au; cyan atoms: Cs. Orange isosurface represents the probability of finding the electron when the hole position (yellow spot) is fixed near a given atomic site.]