

Supporting Information for

Visible light-induced hole transfer in single-nanoplate $\text{Cu}_{1.81}\text{S}$ - CdS heterostructures

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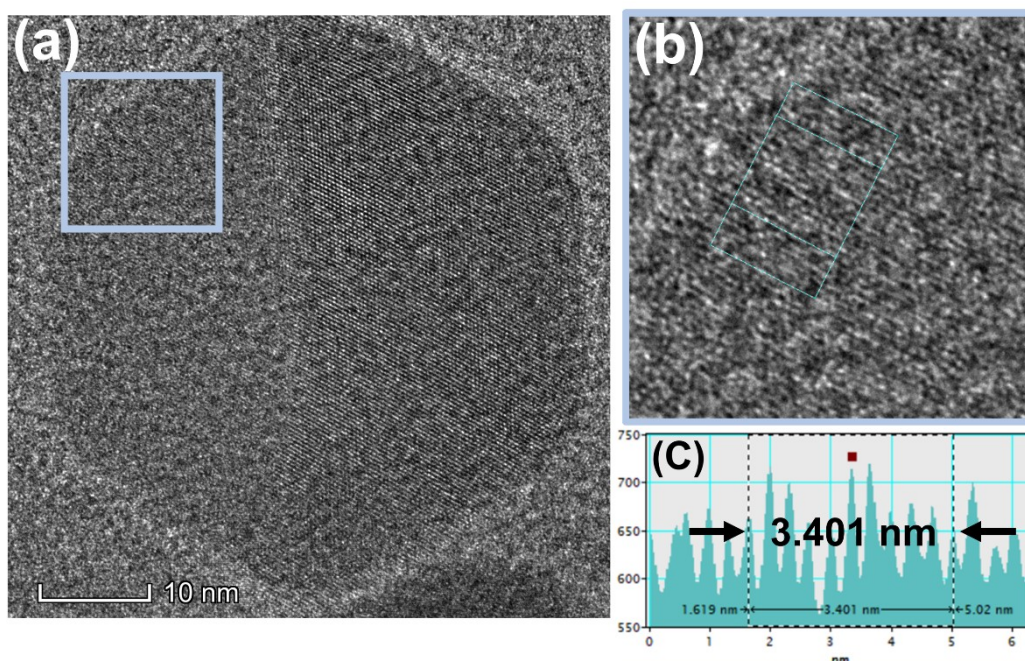


Figure S1: (a) HRTEM images of a single nanoplake $\text{Cu}_{1.81}\text{S}-\text{CdS}$. (b) Lattice fringes in the corresponding blue region. (c) Length of ten lattice fringes.

Density functional theory calculations

Calculations were performed using the Vienna Ab initio Simulation Package (VASP).¹ The Perdew–Burke–Ernzerhof (PBE) standard functional is used as the exchange–correlation functional. A plane-wave cutoff of 400 eV was used for all calculations.² The convergence criteria for the electronic self-consistent iteration and the residual force on each relaxed atom were set to 10^{-4} eV and 0.03 eV/Å, respectively.³ The (002) surface of CdS and the (400) surface of $\text{Cu}_{1.81}\text{S}$ were used for modelling. The crystal structures of CdS and $\text{Cu}_{1.81}\text{S}$ were taken from literature [4] and [5], respectively. A vacuum spacing of 30 Å in the slab was set to separate the surface along a perpendicular direction. A single k-point (Γ -point) was adopted for the Brillouin-zone sampling,⁶ which was appropriate for the slab model with rather large surface unit cell.

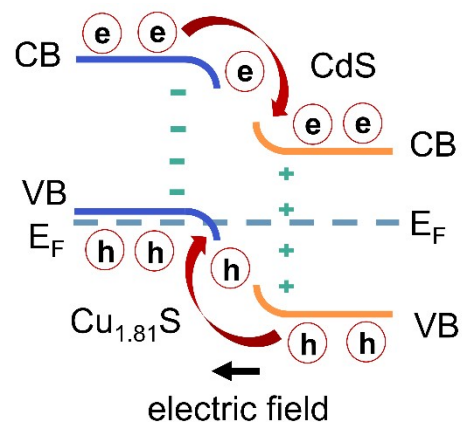


Figure S2: schematic illustration of charge separation at the interface of $\text{Cu}_{1.81}\text{S}$ - CdS .

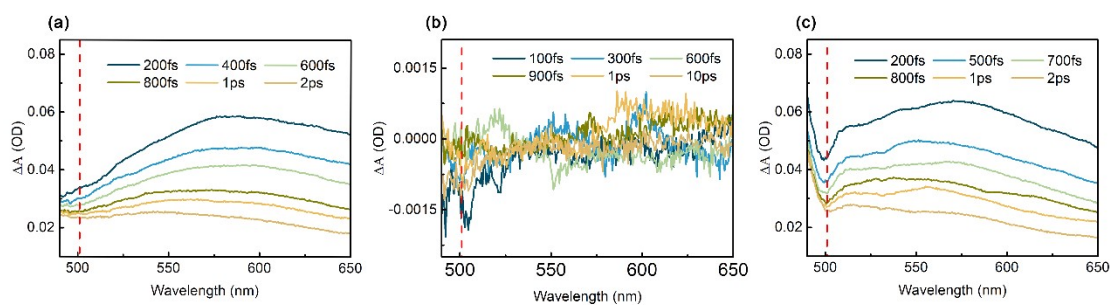


Figure S3. TA spectra of $\text{Cu}_{1.81}\text{S}$ (a), CdS (b), and $\text{Cu}_{1.81}\text{S-CdS}$ (c) were recorded at selected delay times following 1300 nm laser excitation.

Fig. S3 shows the TA spectra of $\text{Cu}_{1.81}\text{S}$, CdS and $\text{Cu}_{1.81}\text{S-CdS}$ after selective excitation of the localized surface plasmon resonance band by a 1300 nm laser. At this point, the CdS nanoplates showed no significant absorption signal, indicating that they were not excited. Whereas, a broad absorption peak can be observed in $\text{Cu}_{1.81}\text{S}$ nanoplates, indicating that copper sulphide is selectively excited. It is noteworthy that a significant dip can be seen in the CdS excitonic peak region after localized surface plasmon resonance excitation. The dip in the TAS to CdS bleaching caused by state-filling⁷ derived from electron transfer from the $\text{Cu}_{1.81}\text{S}$ to CdS phases under 1300 nm laser excitation.⁸

References

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