Electronic Supplementary Information.

Ultrafast charge transfer dynamics pathways in two dimensional MoS_2-graphene heterostructures: A core hole clock approach.

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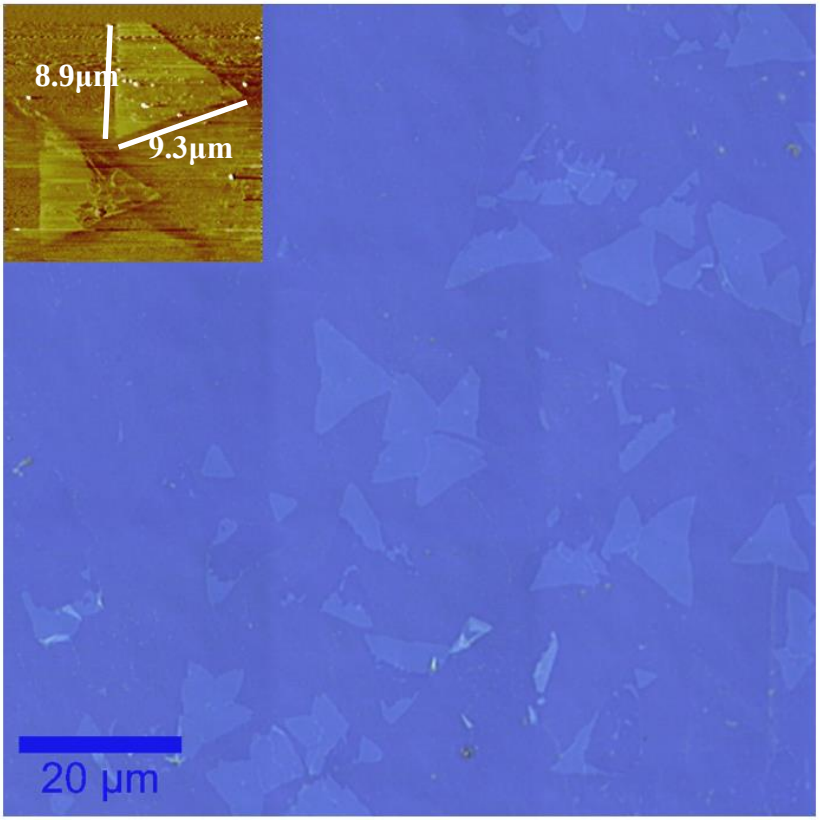


Fig. S1 Optical micrograph of the $MoS_2/SiO_2/Si$ heterostructure. The inset shows the corresponding AFM imagen.

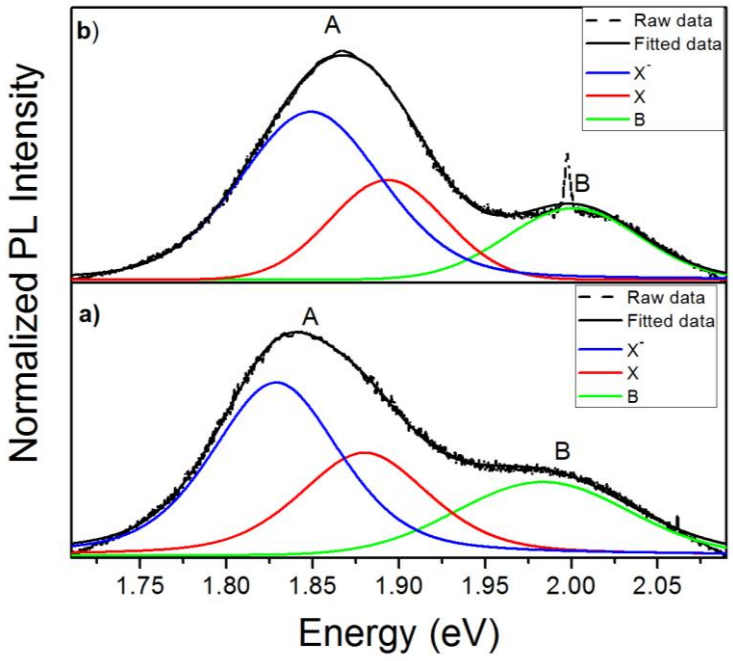


Fig. S2 PL spectra fitting of the: a) $MoS_2/SiO_2/Si$ and b) MoS_2/graphene/SiO_2/Si heterostructures. The A peak was deconvoluted by two contributions labelled as X (blue line) and X^-(red line), while the peak B (green line) was deconvoluted by only one contribution. The fitting was performed using a linear combination of 50% of Gaussian (G) and 50 % of Lorentzian (L) functions.

PL spectra were fitted using a linear combination of Gaussian (G) and Lorentzian (L) functions and showed in figure S2. The quantitative parameters of these fitting were presented in Table S1. The peak A was decomposed in two contributions, which are associated to the exciton (X~ 1.88 eV) and the trion (X^-~ 1.82 eV) excited species, while peak B was fitted by only one contribution[1]. The peak A in both samples is dominated by the trion (electron-coupled to exciton) excited species. From the parameters reported in the table S1 is possible to calculate the relative concentration of the exciton species contributing to A PL peak from the following equation used by Buscema *et al.*[2] :

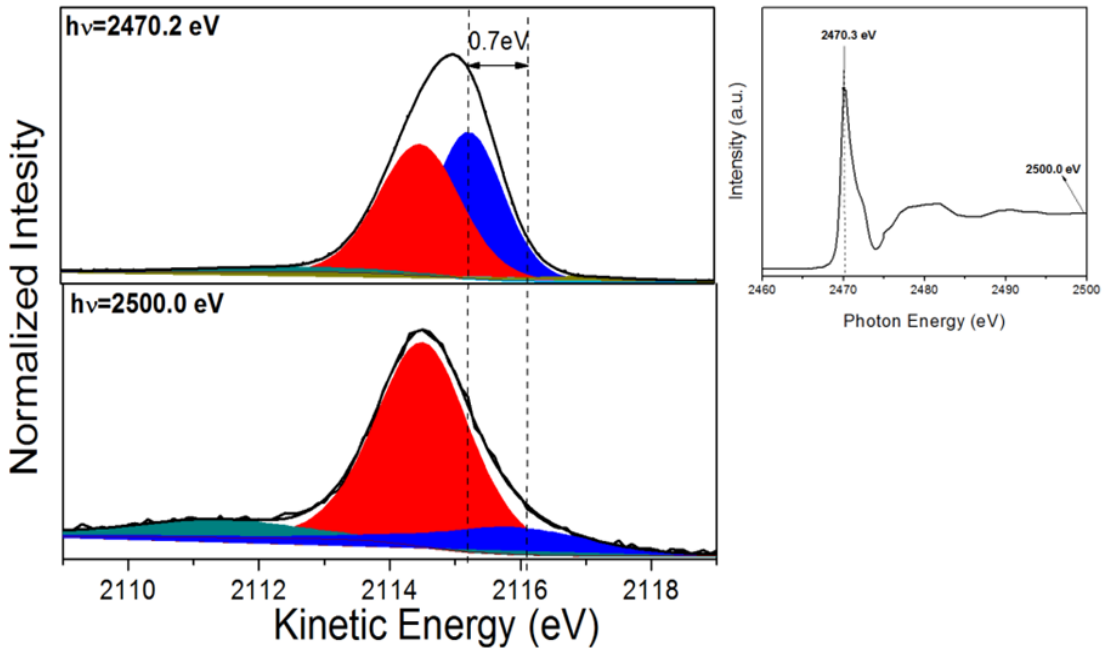
$\gamma=(I_X/(I_X+ I_{X^-})*100)$, where I_X and I_{X^-} represent the intensity of exciton and trion excited species, respectively.

The exciton X percentage in peak A decrease from 39% in $MoS_2/SiO_2/Si$ to 31% in MoS_2/graphene/SiO_2/Si sample, while for the contribution of the trion, the percentage increase from 61% in the $MoS_2/SiO_2/Si$ to 69% in the MoS_2/graphene/SiO_2/Si. The last results means that PL quenching observed for the peak A in the MoS_2/graphene/SiO_2/Si heterostructure is mainly due to the neutral exciton (X) dissociation on MoS_2-graphene interface. Specifically, the exciton dissociation is associated to electron transfer from MoS_2 conduction band to graphene [3].

Table S1 – Fitting parameters of the PL spectra of MoS_2/SiO_2 and MoS_2/graphene/SiO_2 heterostructures.

Peak	MoS_2/SiO_2			MoS_2/graphene/SiO_2		
	Position (eV)	FWHM (eV)	Area (%)	Position (eV)	FWHM (eV)	Area (%)
X^-	1.82	0.09	48	1.85	0.10	55
X	1.88	0.14	30	1.89	0.08	25
B	1.98	0.09	22	2.00	0.09	20

a)



b)

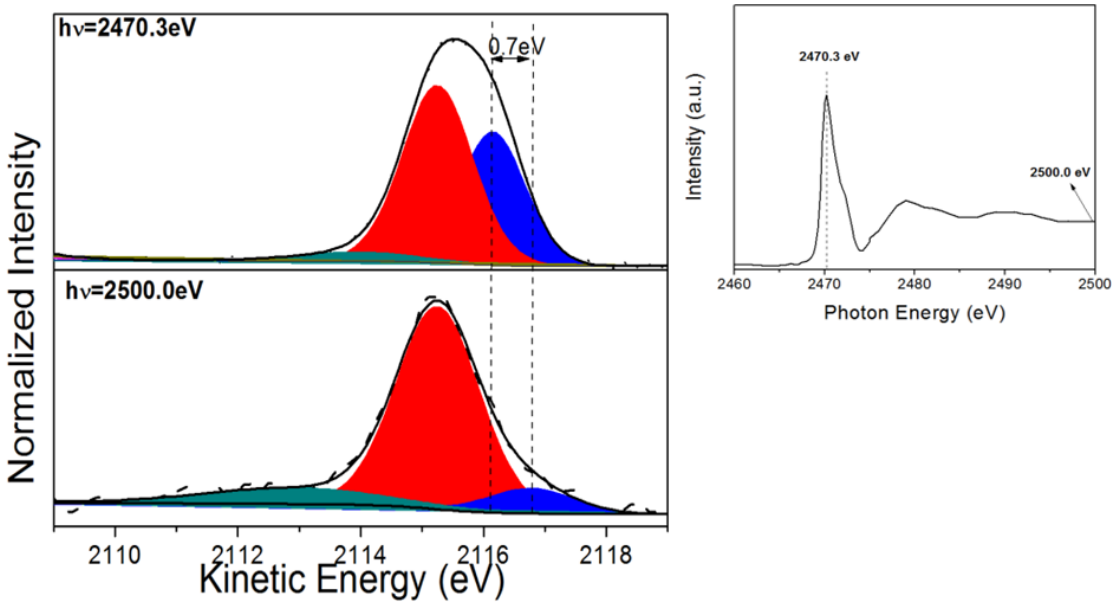


Fig. S3 Determination of spectator shift from S-K $L_{2,3}L_{2,3}$ RAS spectra measured at resonance maximum (2470. 3 eV photon energies) and above S1s ionization potential (2500 eV). a) MoS_2/ SiO_2/Si and b) MoS_2/ graphene/SiO_2/Si heterostructures. The inset shows the respective S K edge NEXAFS spectra with photon energies selected to measure the S-K $L_{2,3}L_{2,3}$ RAS spectra.

The graphene SiO_2/Si fermi level and MoS_2/graphene/SiO_2/Si VBM were determined from the intersection of the linear extrapolation of the leading edge of their respective valence band spectra with the base line.

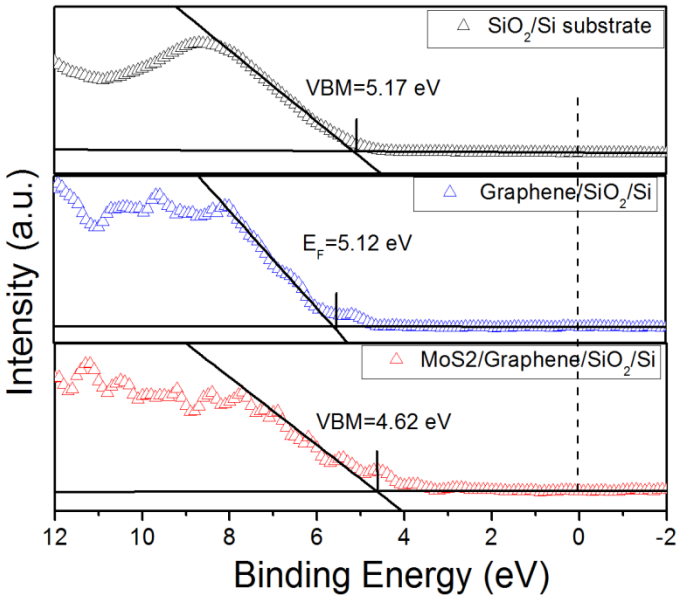


Fig. S4 XPS valence band spectra for SiO_2/Si, graphene/SiO_2/Si, MoS_2/graphene/SiO_2/Si samples.

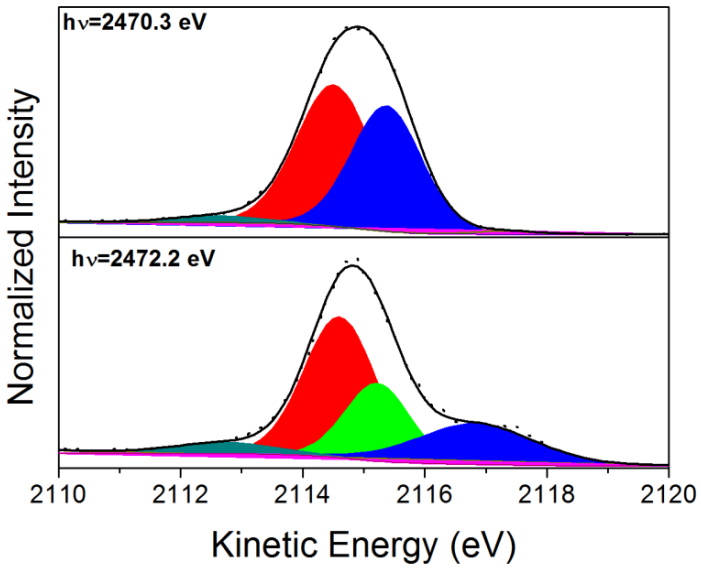


Fig. S5 MoS_2/SiO_2 S-K $L_{2,3}L_{2,3}$ RAS spectra deconvolution in resonant spectator SP1 (blue feature), SP2 (green) and non-resonant NA (red curve) decay channels measured for S1s-$3p_{x,y}$ (2070.3 eV) and S1s-$3p_Z$ (2472.2 eV) transitions, respectively.

References

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