Supporting Information

Observation of Robust Charge Transfer under Strain Engineering in Two-Dimensional MoS₂-WSe₂ Heterostructures

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1. Experimental detail

1.1 Sample preparation: The MoS_2 and WSe_2 monolayer continuous films were purchased from 6 Carbon Technology, Shenzhen. The MoS_2 (WSe_2) film made by chemical vapor deposition (CVD) was firstly coated with a layer of polymethyl methacrylate (PMMA). Then, the PMMA-support MoS_2 (WSe_2) film was transferred to WSe_2 (MoS_2) film on the PET flexible substrate in order to apply a uniaxial strain. The prepared heterostructures were immersed in acetone to remove PMMA, and vacuum annealing at 100 °C for 6 hours to eliminate residual polymer.¹

1.2 Steady-state characterizations: The steady-state absorption spectra and PL spectra were characterized with Shimadzu UV-2550 spectrophotometer and FL-4600, respectively. The Raman spectra were measured by Alpha 300R, where the excitation wavelength of laser was 532 nm and the spot size was around 0.5 mm for Raman measurements.

1.3 Femtosecond broadband TA system: We used a mode-locked Ti: sapphire amplifier to generate 800 nm (repetition rate: 500 Hz) laser pulse with 35 fs pulse width (Solstice, Spectra-Physics). The system split the beam through a 80% (reflection)/20% (transmittance) mirror: one stronger beam of light passed through the TOPAS system to produces 750 nm excitation light; the other was through a 2 mm water, producing a broad-band probe light (400-800 nm). The signals of TA were gathered in a fiber-coupled spectrometer. The dispersion correction of TA data was performed by a chirp program.



Figure S1. (a) Evolution of Raman spectra for MoS_2 -WSe₂ heterostructure from 0% to 1.2% tensile strains. (b) Evolution of the E_{2g}^{1} peak of WSe₂, E_{2g}^{1} and A_{1g} peaks of MoS_2 for MoS_2 -WSe₂ heterostructures as a function of applied tensile strains.



Figure S2. (a) The normalized dynamics of A-, B- and C-exciton for unstrained monolayer MoS_2 . The normalized dynamics of (b) A-exciton (c) B-exciton and (d) C-exciton for monolayer MoS_2 under 0%, 0.4%, 0.8%, and 1.2% strains.



Figure S3. The time-resolved dynamics probed at 649 nm, 652 nm, 656 nm and 676 nm (trion) for unstrained MoS₂. The trion is always appear on the red edge of the A-exciton.^{2,3} It is found that the decay of the A-exciton of MoS_2 (649 nm) is accompanied by the formation of A-trions. It clearly shows that for the time-resolved dynamics probed at 676 nm, there is a signal overlapping between the signals of A-excitons and A-trions.



Figure S4. The normalized dynamics of (a) A-exciton (c) B-exciton (d) A'-exciton (d)

C-exciton for monolayer WSe₂ under 0%, 0.4%, 0.8%, and 1.2% strains.



Figure S5. Typical optical microscopic image for MoS_2 -WSe₂ heterostructures. We choose the area to clearly show the superposition regions in MoS_2 -WSe₂ heterostructures.

Applied strains	A _{1g} of MoS ₂	E _{2g1} of MoS ₂	E _{2g1} of WSe ₂
0%	403.1	384.0	250.8
0.4%	400.5	381.6	249.4
0.8%	399.2	378.6	247.9
1.2%	396.0	376.6	246.5

Table S1. The values of Raman peak under applied strains for monolayer MoS_2 and monolayer WSe_2 .

Applied strains	MoS ₂	WSe ₂
0%	0.62	0.20
0.4%	0.64	0.61
0.8%	0.67	0.88
1.2%	0.79	1.07

Table S2. The relative carrier population ratio of C/(A+B) under applied strains for monolayer MoS_2 and monolayer WSe_2 .

Table S3. The estimated band shrinkage values at K point under applied strains according to the red-shift of A-exciton peak for monolayer MoS_2 , monolayer WSe_2 and MoS_2 -WSe₂ heterostructures, in comparison with unstrained samples.

Applied	MoS ₂	WSe ₂	MoS ₂ -WSe ₂	
strains			MoS ₂	WSe ₂
0.4%	12 meV	7 meV	14 meV	18 meV
0.8%	26 meV	11meV	26 meV	24 meV
1.2%	41 meV	16 meV	26 meV	24 meV

Reference

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