## **Sulfur Isotope Engineering in Heterostructures of Transition**

## **Metal Dichalcogenides**

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**Supplementary Information** 



**Figure S1**: (a-d) Microscopic optical images depicting the growth pattern of  $MoS_2(^{34}S/MoS_2(^{32}S))$ IHS and their (e-h) corresponding PL images under green light.



**Figure S2:** Raman spectra depicting shear and breathing modes,  $E_{2g}^2$  and  $B_{2g}^2$  along with fitting for BL MoS<sub>2</sub>(<sup>32</sup>S), BL MoS<sub>2</sub>(<sup>34</sup>S) and IHS.

Sample	Raman Modes	Raman shift (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )	Integral Intensity (cps.cm <sup>-1</sup> )
BL MoS <sub>2</sub> ( <sup>32</sup> S)	$E_{2g}^{2}$	21	3	4201
	$B_{2g}^{2}$	39	10	15019
BL MoS <sub>2</sub> ( <sup>34</sup> S)	$E_{2g}^{2}$	22	3	2410
	$B_{2g}^2$	38	10	10025
IHS	$E_{2g}^{2}$	21	3	1037
	$B_{2g}^{2}$	38	9	3086

**Table S1:** Fit parameters of  $E_{2g}^2$  and  $B_{2g}^2$  from the fitting of **Figure S3.** 



**Figure S3**: Optical images of BL  $MoS_2(^{32}S)$  exhibiting AA and AB stackings along with their corresponding low-frequency Raman modes.



**Figure S4**: (a) and (b) shows the optical images of two IHS along with their Raman mapping across the sum of shear (S) mode in (c) and (d), respectively.



**Figure S5:** Spatial map of  $MoS_2(^{32}S)$  and  $MoS_2(^{34}S)$  depicting IHJ along with two peak fittings of the Raman spectra from the position depicted in the cursor.

Sample	Raman Modes	Raman shift (cm <sup>-1</sup> )	FWHM (cm <sup>-1</sup> )
	$E^{'}$	383	3
MoS <sub>2</sub> ( <sup>32</sup> S)	$A'_1$	404	7
	2LA	453	24
	E'	377	4
MoS <sub>2</sub> ( <sup>34</sup> S)	$A'_1$	393	4
	2LA	447	25
	E'	377	6
	E'	382	4
IHJ	$A'_1$	395	4
	$A'_1$	402	10
	2LA	449	28
	$E_{2g}^1$	379	6
	$A_{1g}$	394	4
IHS	$A_{1g}$	400	5
	$A_{1g}$	404	8
	2LA	448	25

**Table S2**: Fitting parameters for the Raman spectra of ML  $MoS_2(^{32}S)$ , ML  $MoS_2(^{34}S)$ , IHJ, and IHS are shown in **Figure 3(d-g**).



**Figure S6**: PL spectra along with fitting in yellow line and deconvolution of *A* and *B* excitons for (a) ML  $MoS_2(^{32}S)$  and (b) ML  $MoS_2(^{34}S)$ .

Sample	Exciton	Exciton Energy (eV)	FWHM (meV)	Integral Intensity (cps.eV)
BL MoS <sub>2</sub> (32S)	А	1.82	71	381
	В	1.96	181	336
BL MoS <sub>2</sub> ( <sup>34</sup> S)	А	1.84	83	519
	В	1.97	138	760
IHS	А	1.82	72	40
	В	1.96	140	147

**Table S3**: Fitting parameters for the PL spectra of BL MoS<sub>2</sub>(<sup>32</sup>S), BL MoS<sub>2</sub>(<sup>34</sup>S), and IHS in **Figure 5**.



**Figure S7:** Narrow range scaled PL Mapping of (a-b) A exciton and (c-d) B exciton in two different IHS correlating the heterogeneous stacking indicated by Raman mapping of shear mode in **Figure S4**. (e) Single PL spectra taken from AB and AA stacking zone of (b).