Supplementary Information

Band Edge Tailoring in Few-layer Two-dimensional Molybdenum Sulfides/Selenides Alloys

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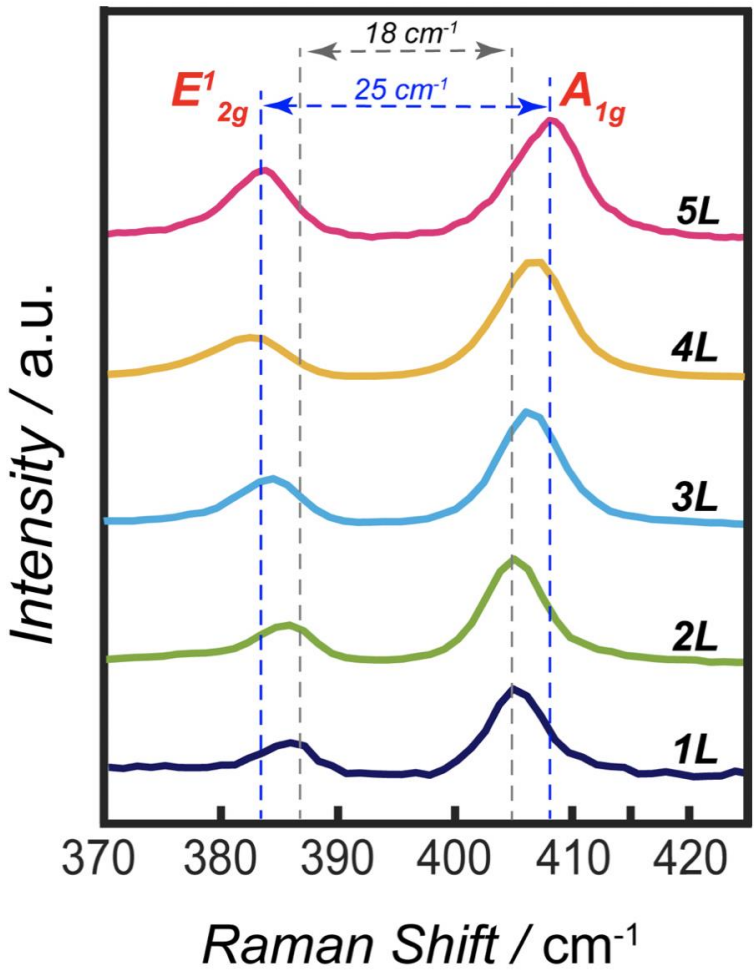


Figure S1. Raman characterizations of MOCVD-grown MoS_2 on 4-inch SiO_2/Si substrate by using 514 nm line. The Raman spectra of different locations with various thicknesses on MoS_2 sample. The 1L and 4L MoS_2 correspond to the location (b) and (c) position as shown in the Figure 1a.

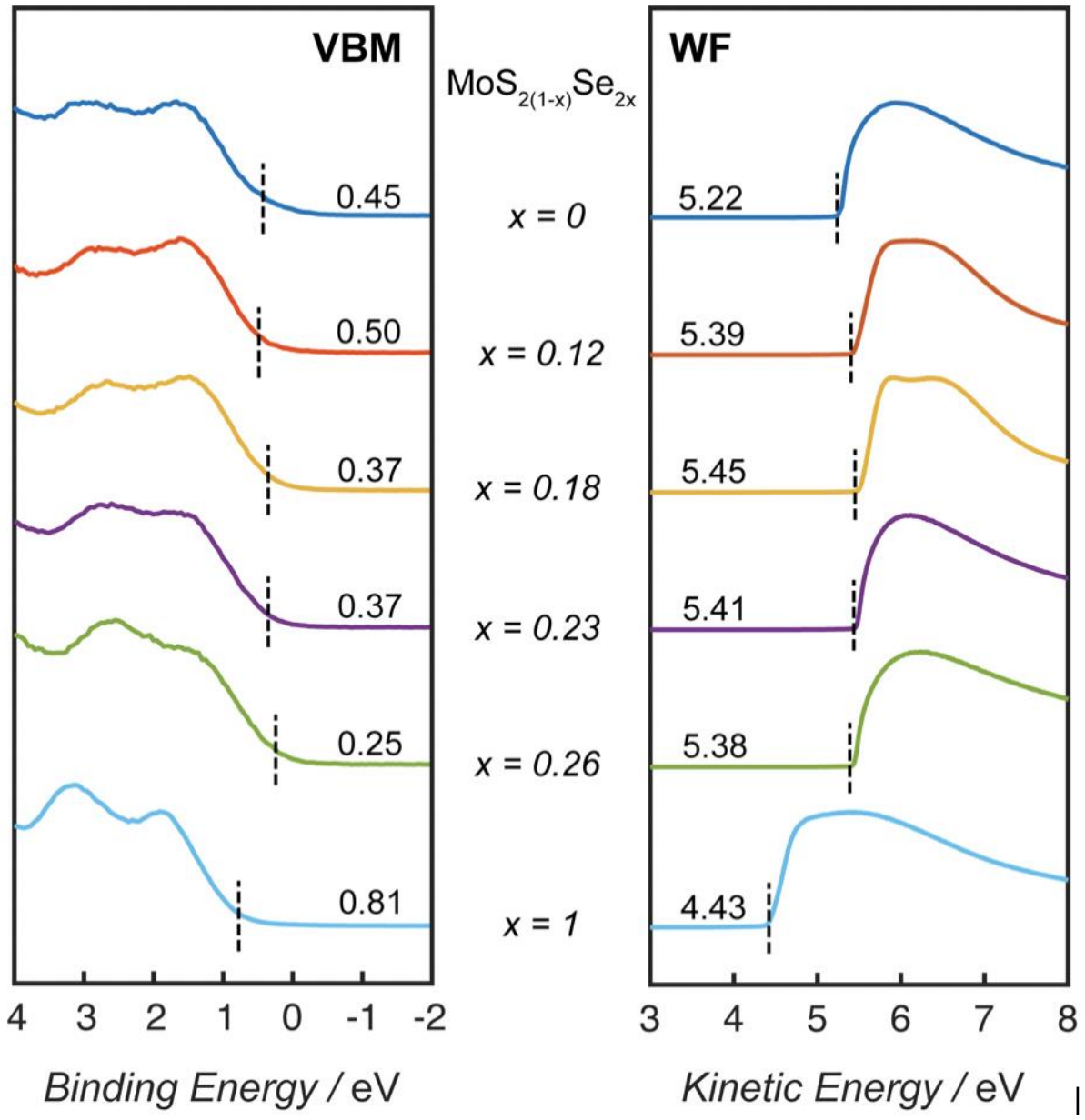


Figure S2. Valence band and work function spectra measured by XPS. The intersection of two lines indicates the valence band maximum of each sample, which is relative to fermi level (E_F for E_B =0).

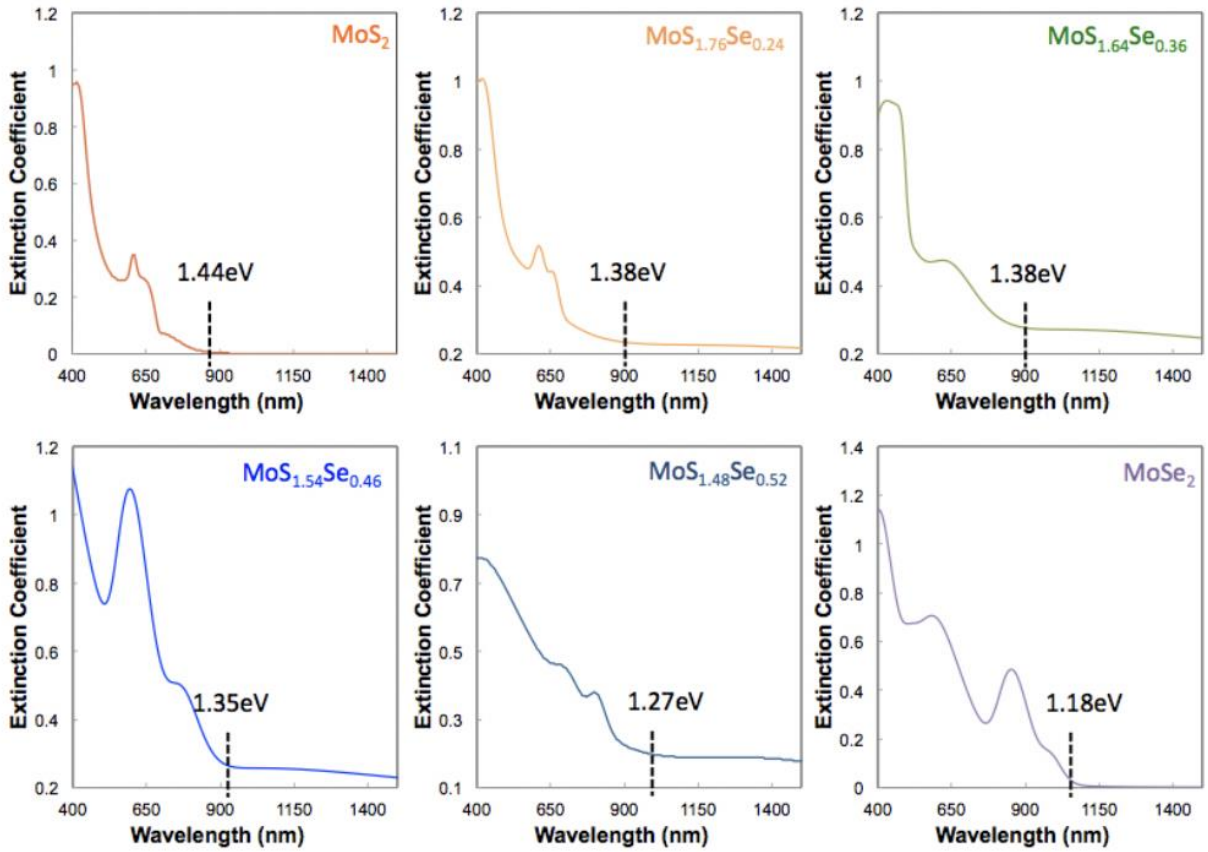
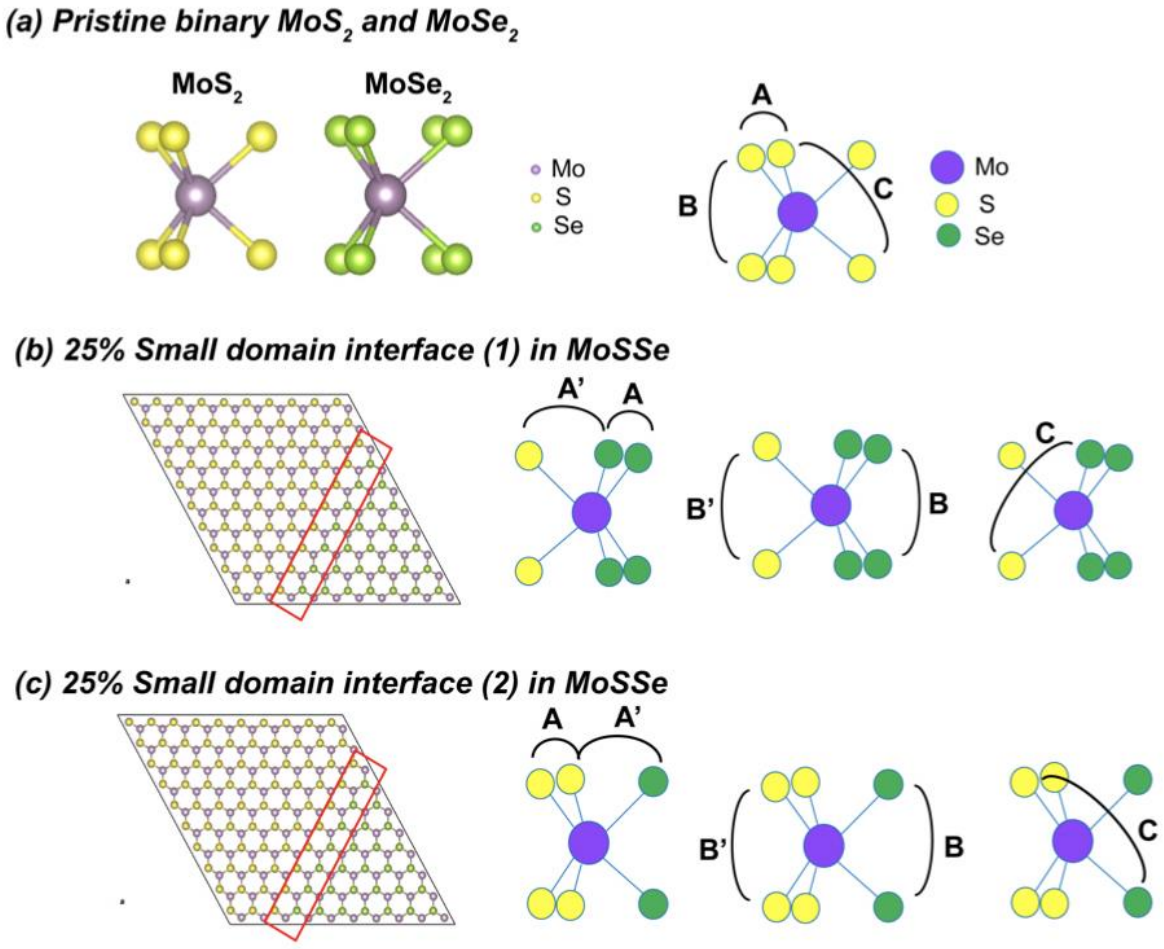


Figure S3. Extinction coefficient of different $MoS_{2(1-x)}Se_{2x}$ samples. The dash lines indicate the optical band gaps of each sample.



(c) Comparison of calculated bond angles

	MoS_2	$MoS_{1.5}Se_{0.5}$ (Interface 1)	$MoS_{1.5}Se_{0.5}$ (Interface 2)	$MoSe_2$
A	81.89	78.42	82.62	81.37
A'		79.67	79.37	
B	81.65 (S)	85.83 (Se)	84.4 (Se)	82.35(Se)
B'		82.74 (S)	82.24 (S)	
C	135.54	137.68	134.35	135.78

Figure S4. (a-c) Simulated bond angles of pristine MoS_2, MoSSe and $MoSe_2$ between various bonds, such as S-S, Se-Se, and S-Se in small domain case (d) comparison of calculated bond angles in various compounds.

Table S1. All the chemical compositions of $MoS_{2(1-x)}Se_{2x}$ in this work.

Averaged chemical compositions of $MoS_{2(1-x)}Se_{2x}$ (with error bar)			
Sample	x value	S	Se
$MoS_{2\pm0.01}$	0	2±0.01	0
$MoS_{1.76\pm0.01}Se_{0.24\pm0.06}$	x=0.12	1.76±0.01	0.24±0.00
$MoS_{1.64\pm0.003}Se_{0.36\pm0.04}$	x=0.18	1.64±0.05	0.36±0.01
$MoS_{1.54\pm0.04}Se_{0.46\pm0.2}$	x=0.23	1.54±0.03	0.46±0.05
$MoS_{1.48\pm0.03}Se_{0.52\pm0.04}$	x=0.26	1.48±0.03	0.52±0.04
$MoSe_{2\pm0.1}$	x=1	0	2±0.06