Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Lowering the Schottky barrier height of G/WSSe van der Waals heterostructures by changing the interlayer coupling and applying external biaxial strain

W.X. Zhang,[1] Y. Yin,[1] C. He[2] *

[1] School of Materials Science and Engineering, Chang'an University, Xi'an 710064, China;

[2] State Key Laboratory for Mechanical Behavior of Materials, School of Materials Science and Engineering, Xi'an Jiaotong University, Xi'an 710049, China.

* Corresponding Author: hecheng@mail.xjtu.edu.cn (C. He)

Table S1 Φ_{TB}, W_{TB} and C values of G/SWSe heterostructure at different interlayer distances.

interlayer distance of G/SWSe	Φ_{TB}	W_{TB}	C
2.5 Å	7.63	1.33	13.58
2.7 Å	8.55	1.50	19.19
2.9 Å	8.96	1.71	26.31
3.1 Å	9.56	1.91	34.77
3.3 Å	9.96	2.12	44.77
3.5 Å	10.12	2.29	52.99
3.7 Å	10.29	2.50	64.31
3.9 Å	10.29	2.70	74.72
4.1 Å	10.38	2.85	84.02
4.3 Å	10.54	3.10	101.22
4.5 Å	10.46	3.28	112.70

Table S2 Φ_{TB}, W_{TB} and C values of G/SWSe heterostructure under different external biaxial strains.

strains of G/SWSe	Φ_{TB}	W_{TB}	C
-8%	9.74	2.18	46.20
-6%	9.90	2.24	49.86
-4%	9.98	2.28	51.64
-2%	10.06	2.28	52.09
0%	10.06	2.24	50.68
2%	10.06	2.34	55.15
4%	10.06	2.38	56.81
6%	10.06	2.34	55.15
8%	10.06	2.38	56.81

Table S3 Φ_{TB}, W_{TB} and C values of G/SeWS heterostructure at different interlayer distances.

interlayer distance of G/SeWS	Φ_{TB}	W_{TB}	C
2.5 Å	6.8	1.22	10.14
2.7 Å	7.56	1.49	16.72
2.9 Å	8.13	1.63	21.55
3.1 Å	8.81	1.89	31.60
3.3 Å	9.13	2.07	38.95
3.5 Å	9.38	2.30	49.55
3.7 Å	9.55	2.47	58.37
3.9 Å	9.71	2.65	68.06
4.1 Å	9.88	2.88	81.92
4.3 Å	10.05	3.09	95.81
4.5 Å	9.96	3.31	109.35

Table S4 Φ_{TB}, W_{TB} and C values of G/SeWS heterostructure under different external biaxial strains.

strains of G/SeWS	Φ_{TB}	W_{TB}	C
-8%	9.08	2.11	40.53
-6%	9.16	2.14	42.07
-4%	9.16	2.14	42.08
-2%	9.25	2.18	43.87
0%	9.32	2.21	45.50
2%	9.57	2.24	48.21
4%	9.57	2.28	49.55
6%	9.41	2.31	50.21
8%	9.57	2.34	52.46

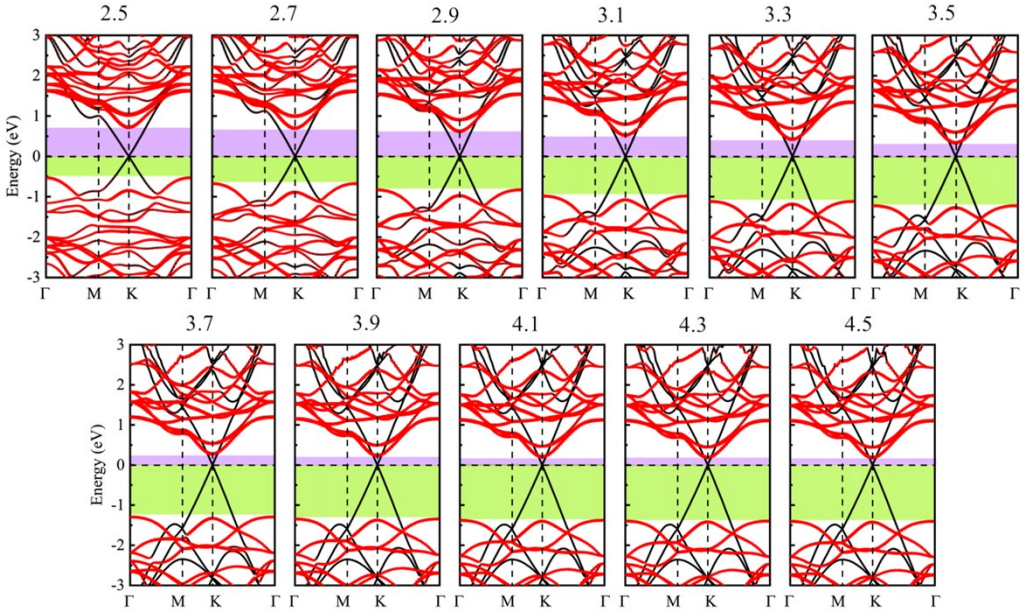

Fig. S1. Band structures of the G/SWSe heterostructure with different interlayer distances from 2.5 Å to 4.5 Å.

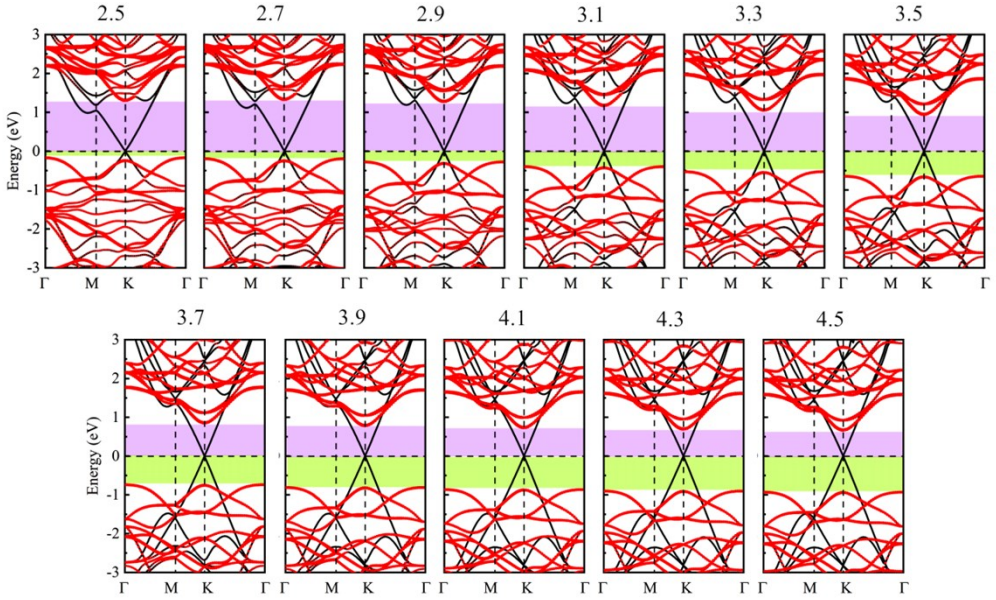

Fig. S2. Band structures of the G/SeWS heterostructure with different interlayer distances from 2.5 Å to 4.5 Å.

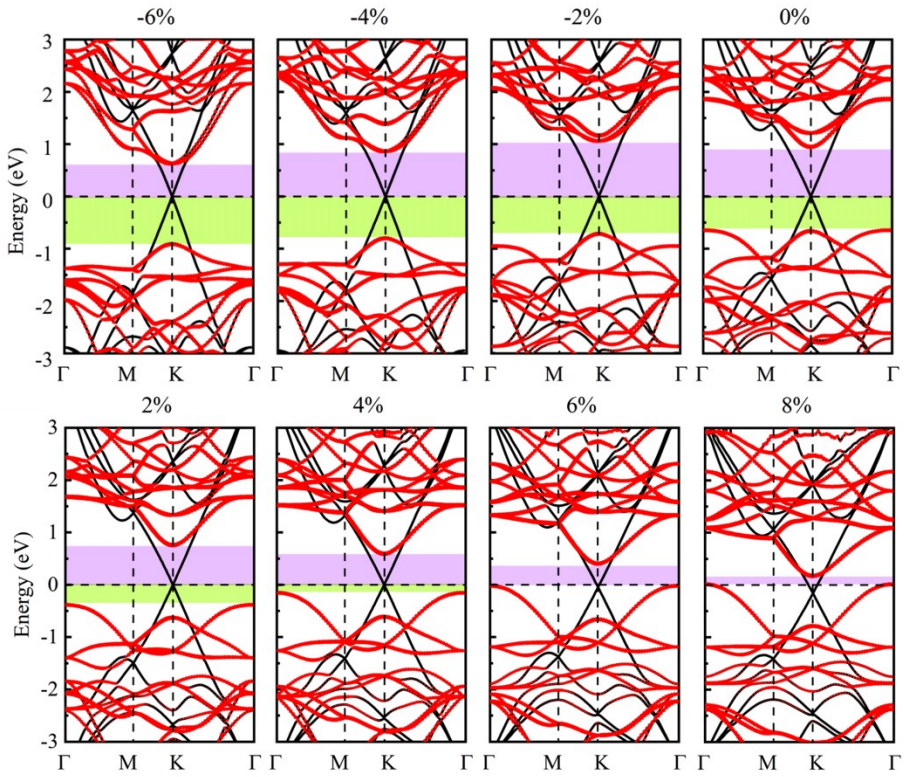

Fig. S3. Band structures of the G/SeWS heterostructure under external biaxial strains from −6% to +8%.

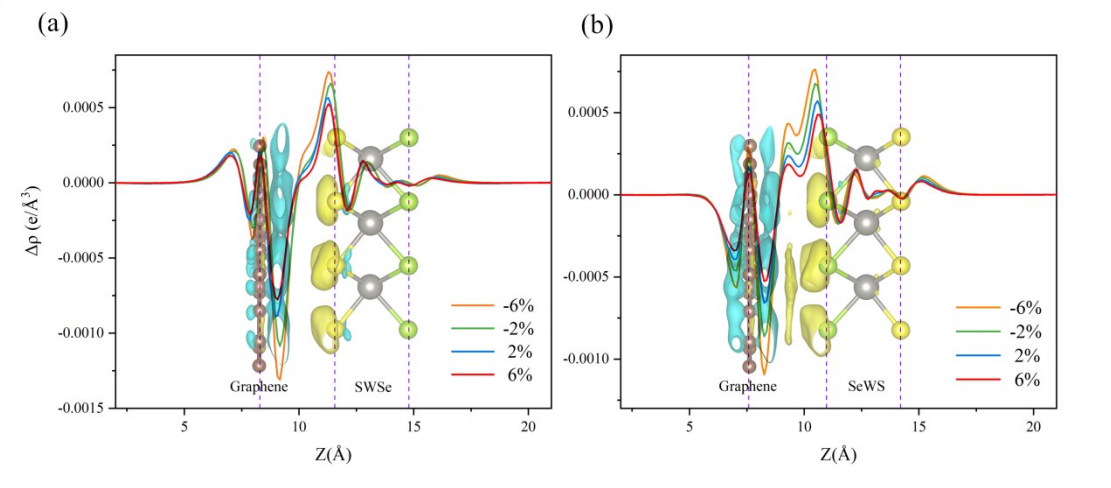

Fig. S4. Charge density difference with an isovalue of 0.001 e/Å^3 and the planar averaged charge density difference for (a) G/SWSe heterostructure and (b) G/SeWS heterostructure with the other relevant external biaxial strains.

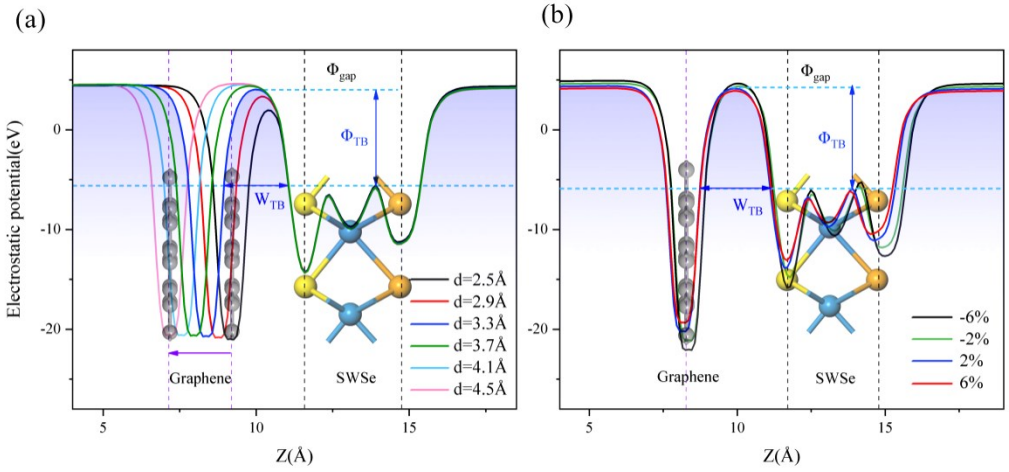

Fig. S5. Effective electrostatic potential profile of G/SWSe heterostructure with the other relevant (a) interlayer distance and (b) external biaxial strains.

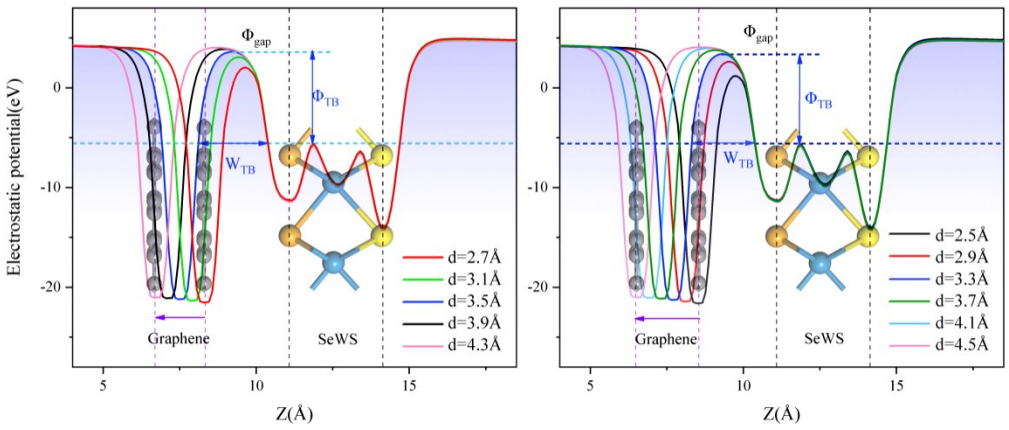

Fig. S6. Effective electrostatic potential profile of G/SeWS heterostructure with different interlayer distance.

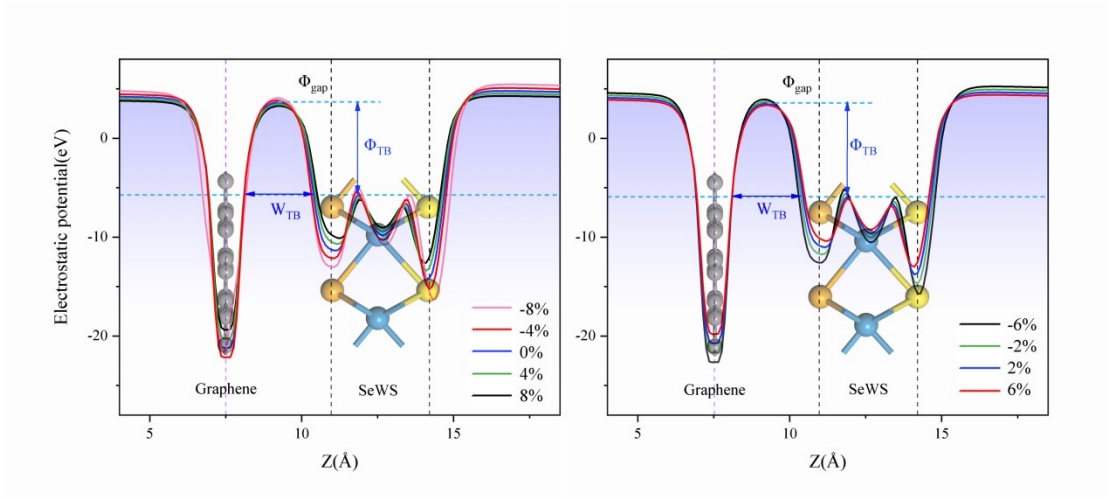

Fig. S7. Effective electrostatic potential profile of G/SeWS heterostructure with different external biaxial strains.