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

Supplementary Information

Structural, Electronic and Optical Properties of four α-Se-based Heterostructures with Hyperbolic Characteristics

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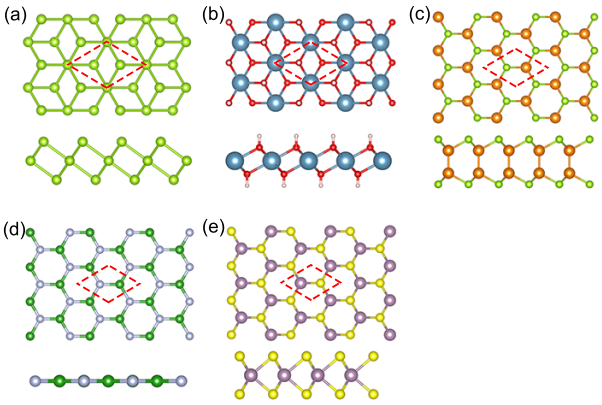

Figure S 1: (Color online). (a)-(e) Optimized structure of α-Se, $Ca(OH)_2$, GaSe, h-BN and MoS_2 monolayers, respectively.

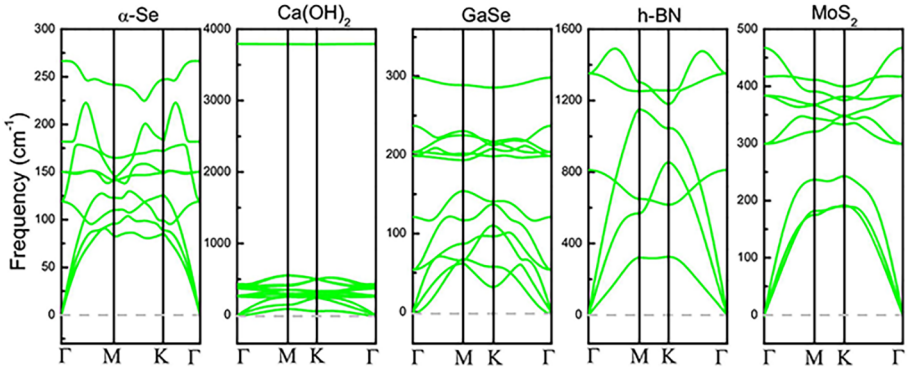

Figure S 2: (Color online). (a)-(e) The calculated phonon dispersion curves of α-Se, $Ca(OH)_2$, GaSe, h-BN and MoS_2 monolayers, respectively.

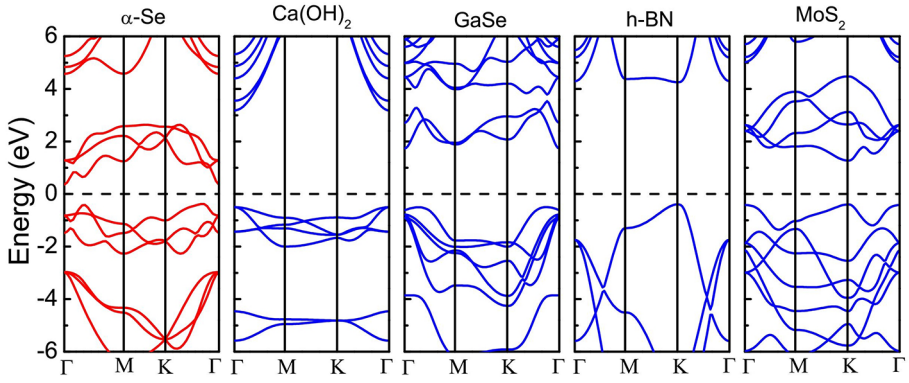

Figure S 3: (Color online). (a)-(e) The calculated electronic band structures of α-Se, $Ca(OH)_2$, GaSe, h-BN and MoS_2 monolayers with PBE method, respectively.

Table S I: The calculated lattice constants (Å), band gap (eV) and band gap type of α-Se, $Ca(OH)_2$, GaSe, h-BN and MoS_2 monolayers, respectively

structure	α-Se	$Ca(OH)_2$	GaSe	h-BN	MoS_2
Lattice (Å)	3.72	3.62	3.82	2.51	3.18
E_g (eV)	0.73	3.68	2.23	4.65	1.68
Band gap type	Indirect	Direct	Indirect	Direct	Direct

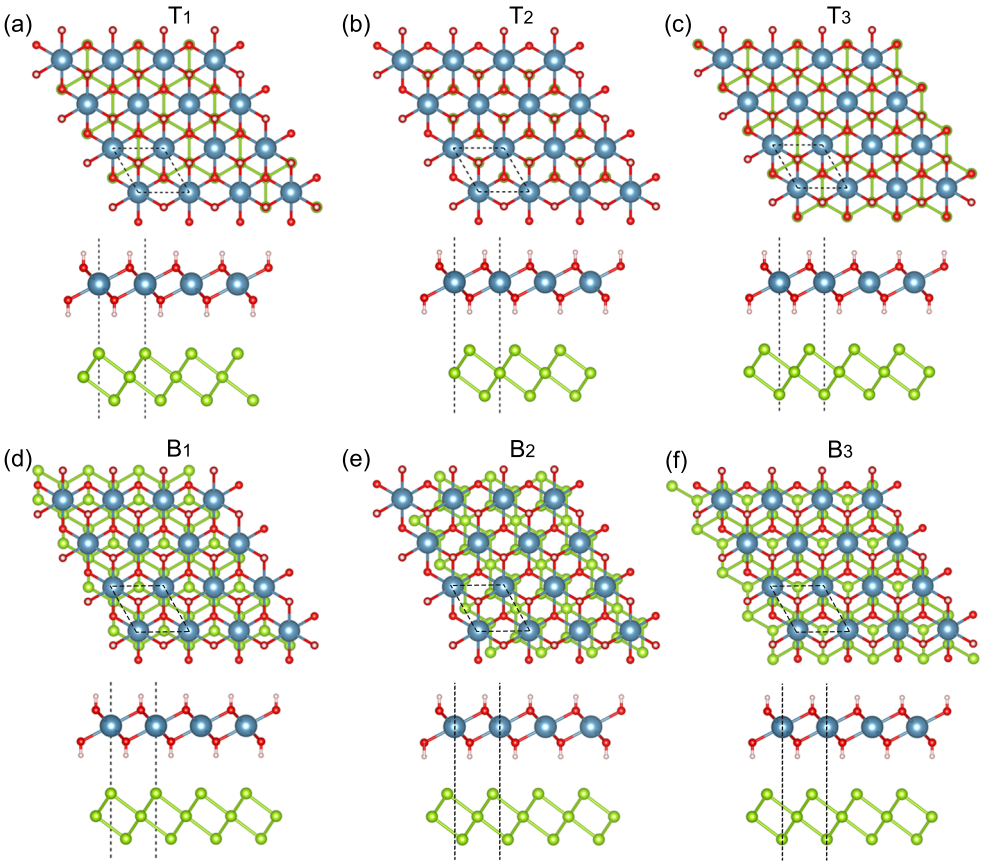

Figure S 4: (Color online). Top and side views of α-Se/$Ca(OH)_2$ heterobilayer with six types of stacking configurations: (a) T_1, (b) T_2, (c) T_3, (d) B_1, (e) B_2 and (f) B_3. The black dashed lines represent the unit cell.

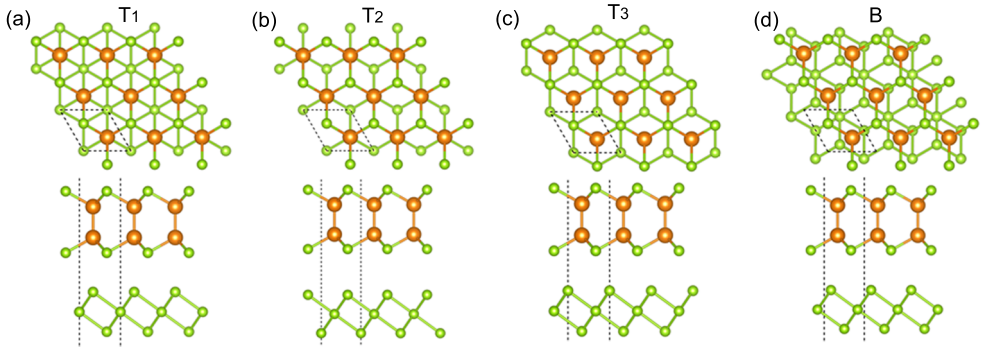

Figure S 5: (Color online). Top and side views of α-Se/GaSe heterobilayer with four types of stacking configurations: (a) T_1, (b) T_2, (c) T_3 and (d) B. The black dashed lines represent the unit cell.

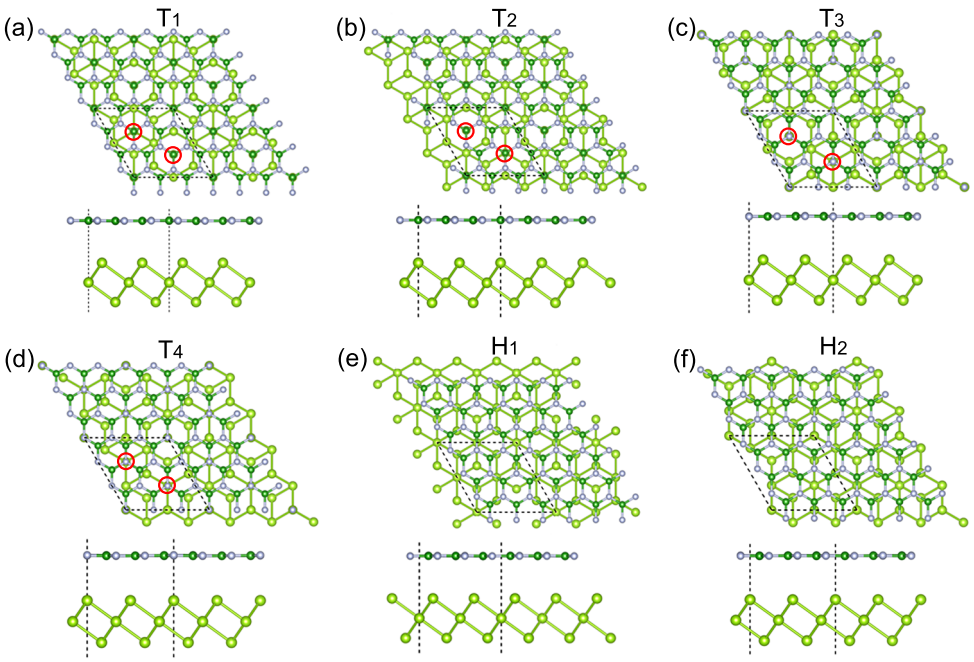

Figure S 6: (Color online). Top and side views of α-Se/h-BN heterobilayer with four types of stacking configurations: (a) T_1, (b) T_2, (c) T_3, (d) T_4, (e) H_1 and (f) H_2. The black dashed lines represent the unit cell.

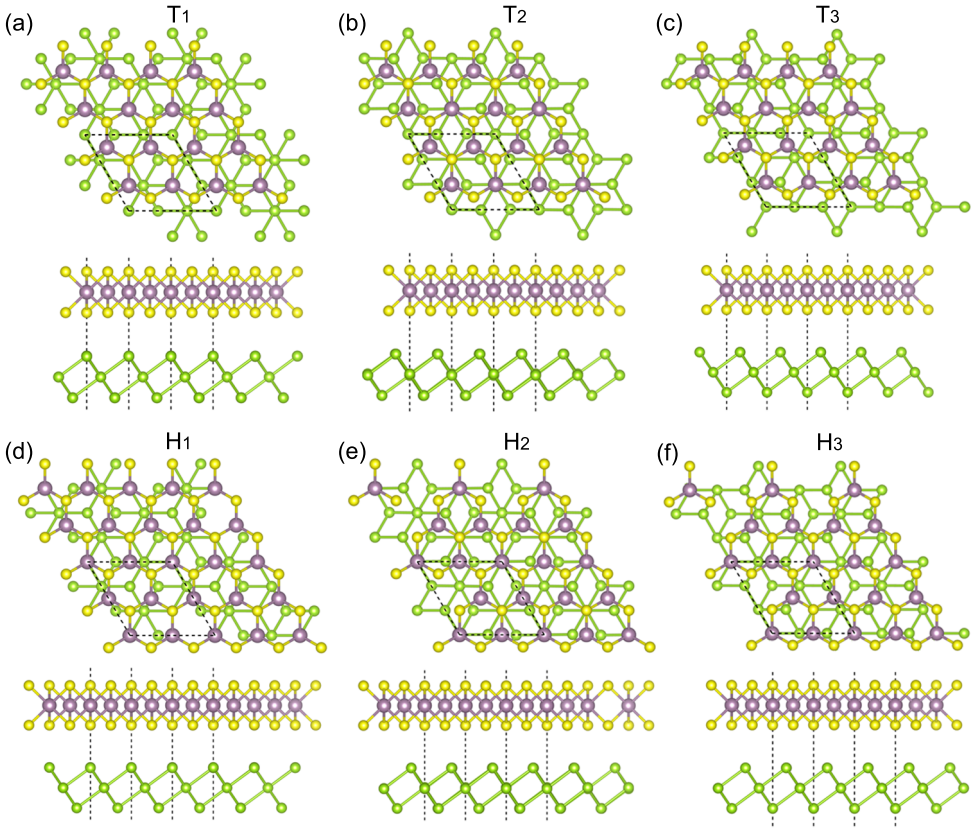

Figure S 7: (Color online). Top and side views of α-Se/MoS_2 heterobilayer with four types of stacking configurations: (a) T_1, (b) T_2, (c) T_3, (d) H_1, (e) H_2 and (f) H_3. The black dashed lines represent the unit cell.

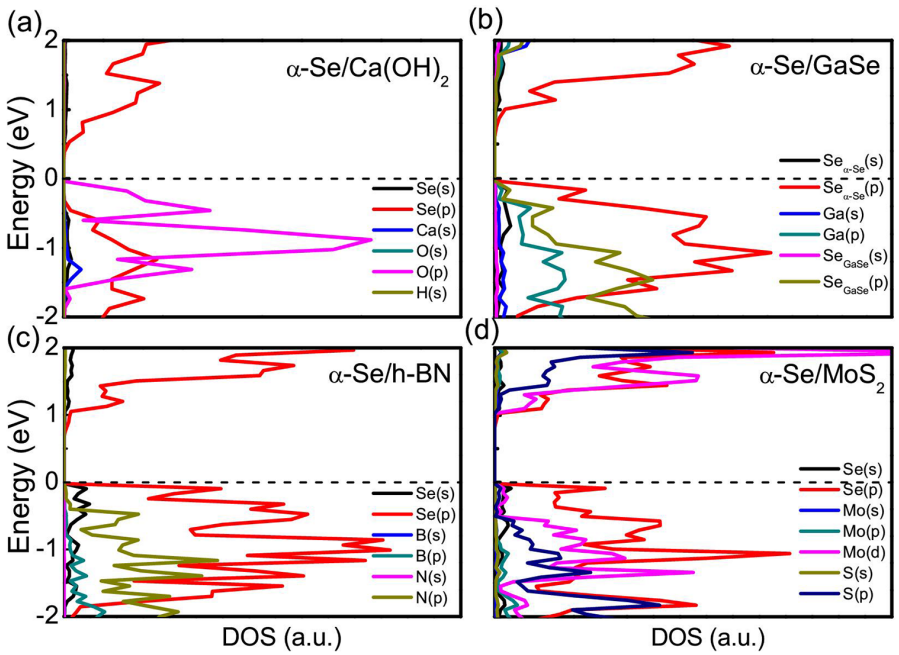

Figure S 8: (Color online). (a)-(d) The projected density of states (PDOS) of α-Se/$Ca(OH)_2$, α-Se/GaSe, α-Se/h-BN and α-Se/MoS_2 VDWHs, respectively.

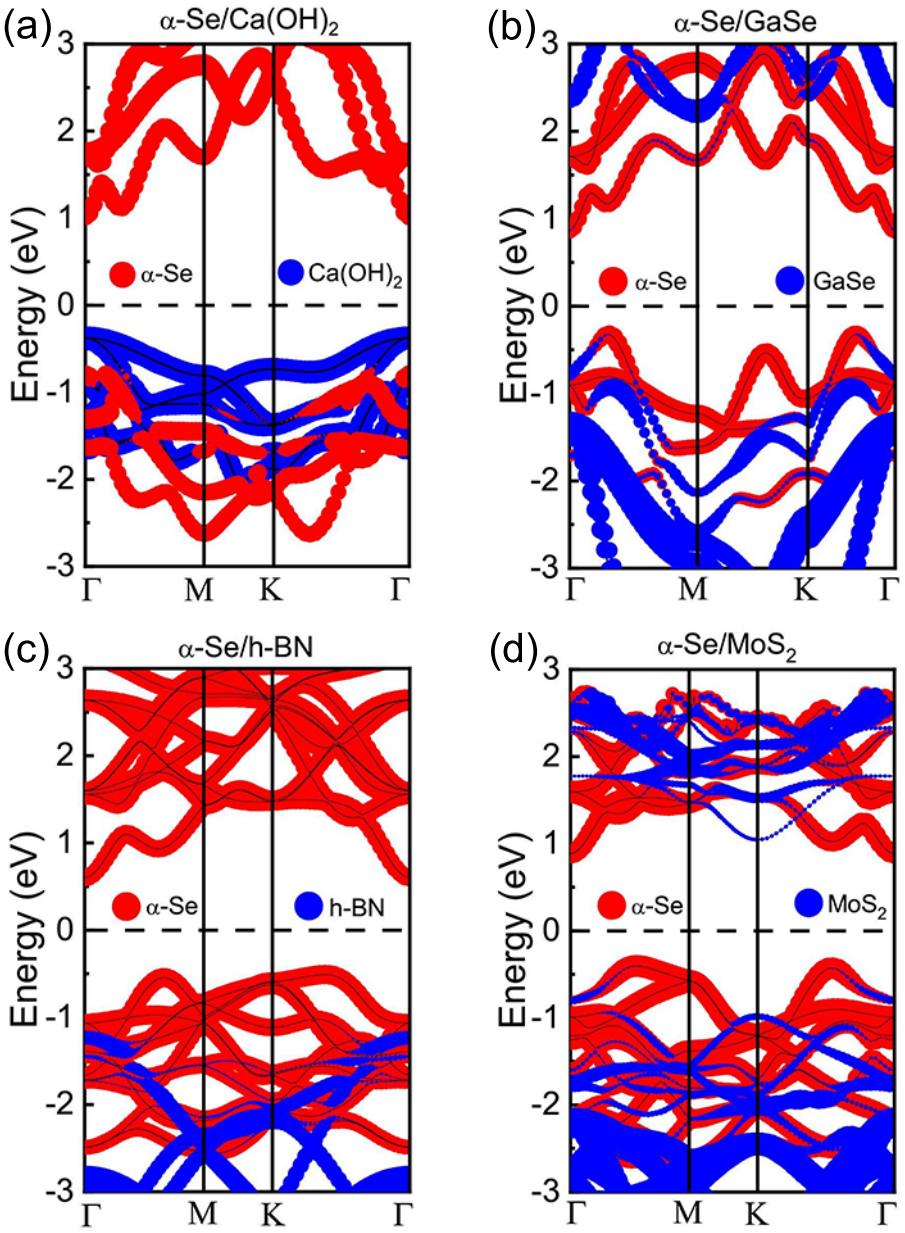

Figure S 9: (Color online). (a)-(d) The projected band structures of (a) α-Se/$Ca(OH)_2$, (c) α-Se/GaSe, (e) α-Se/h-BN and (g) α-Se/MoS_2 VDWHs. The partial charge densities of the VBM and CBM for (b) α-Se/$Ca(OH)_2$, (d) α-Se/GaSe, (f) α-Se/h-BN and (h) α-Se/MoS_2 VDWHs obtained by HSE06 functional, respectively.

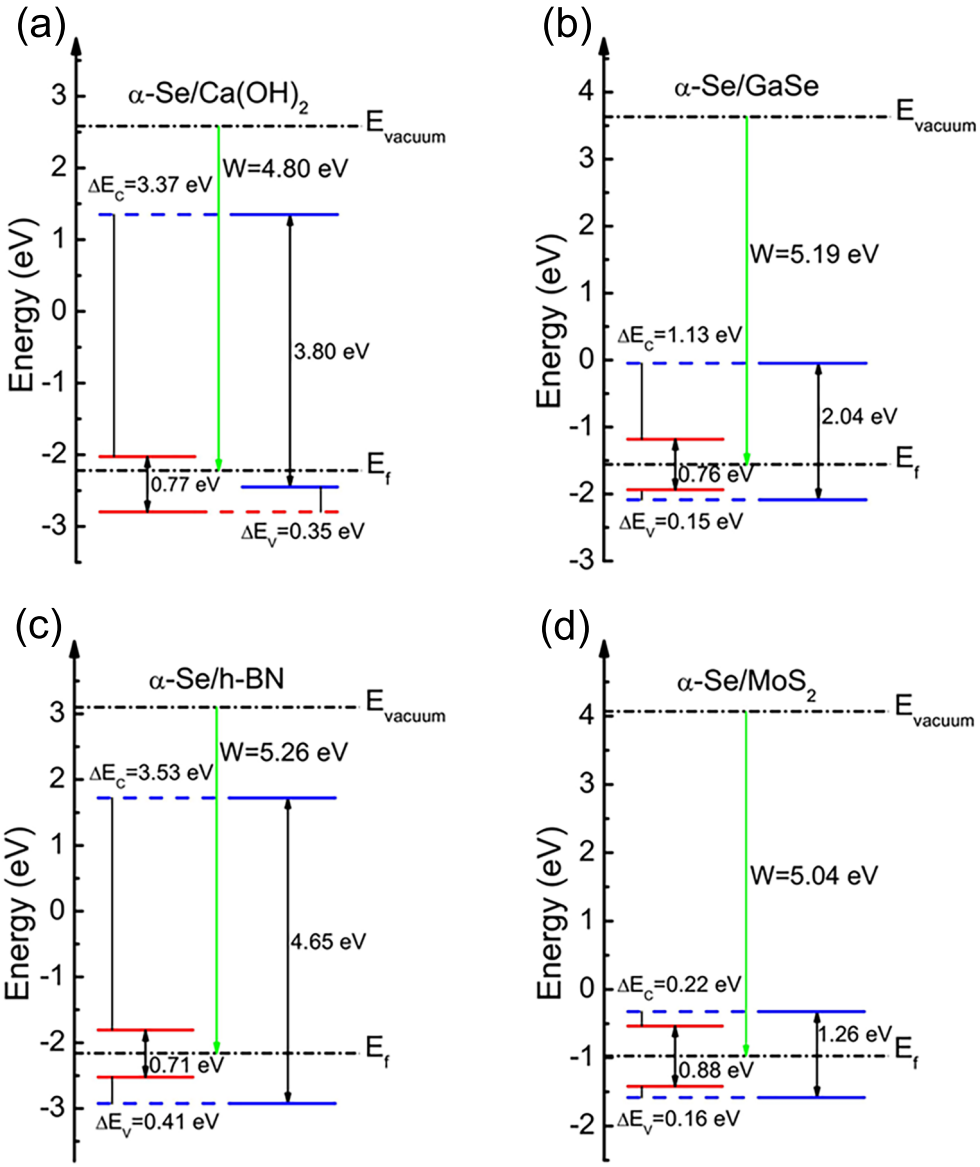

Figure S 10: (Color online). (a)-(d) The band alignment of α-Se/$Ca(OH)_2$, α-Se/GaSe, α-Se/h-BN and α-Se/MoS_2 VDWHs, respectively.

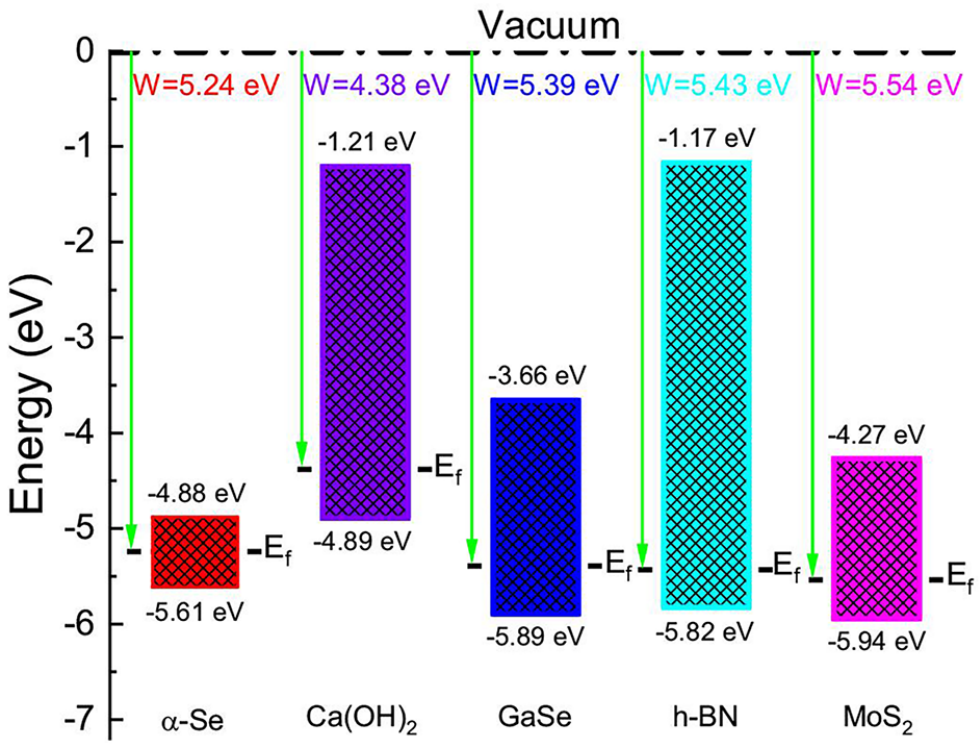

Figure S 11: (Color online). (a)-(e) The band-edge position of α-Se, $Ca(OH)_2$, GaSe, h-BN and MoS_2 monolayers, respectively.

Table S II: The calculated effective mass for electrons and holes of α-Se/$Ca(OH)_2$, α-Se/GaSe, α-Se/h-BN and α-Se/MoS_2 VDWHs along the x and y directions.

VDWH	m_e^x (m_0)	m_e^y (m_0)	m_h^x (m_0)	m_h^y (m_0)
α-Se/$Ca(OH)_2$	0.13	0.11	3.57	2.27
α-Se/GaSe	0.14	0.12	0.66	1.25
α-Se/h-BN	0.11	0.10	0.47	1.49
α-Se/MoS_2	0.13	0.14	1.42	0.49

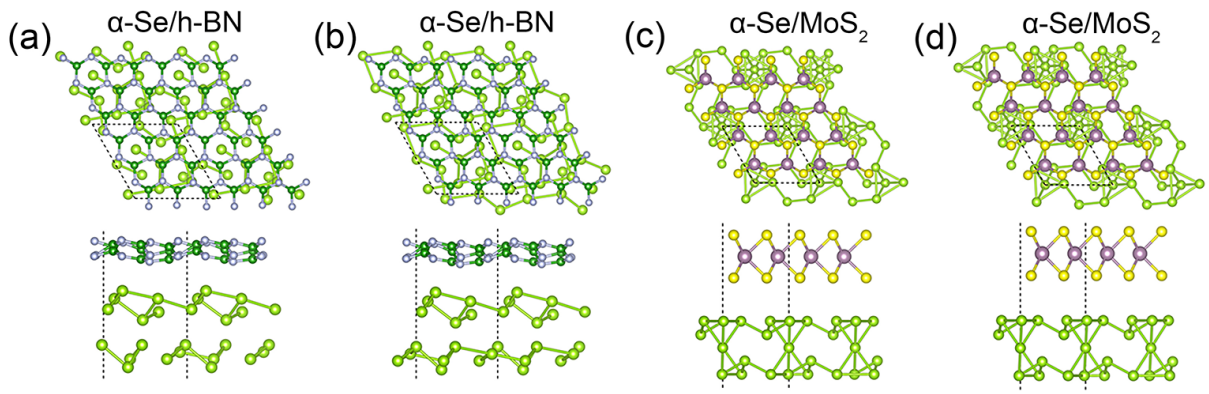

Figure S 12: (Color online). The structures of α-Se/h-BN VDWH when the compressive strain is (a) -9% and (b) -10%, respectively. The structures of α-Se/MoS_2 VDWH when the compressive strain is (c) -8% and (d) -10%, respectively.

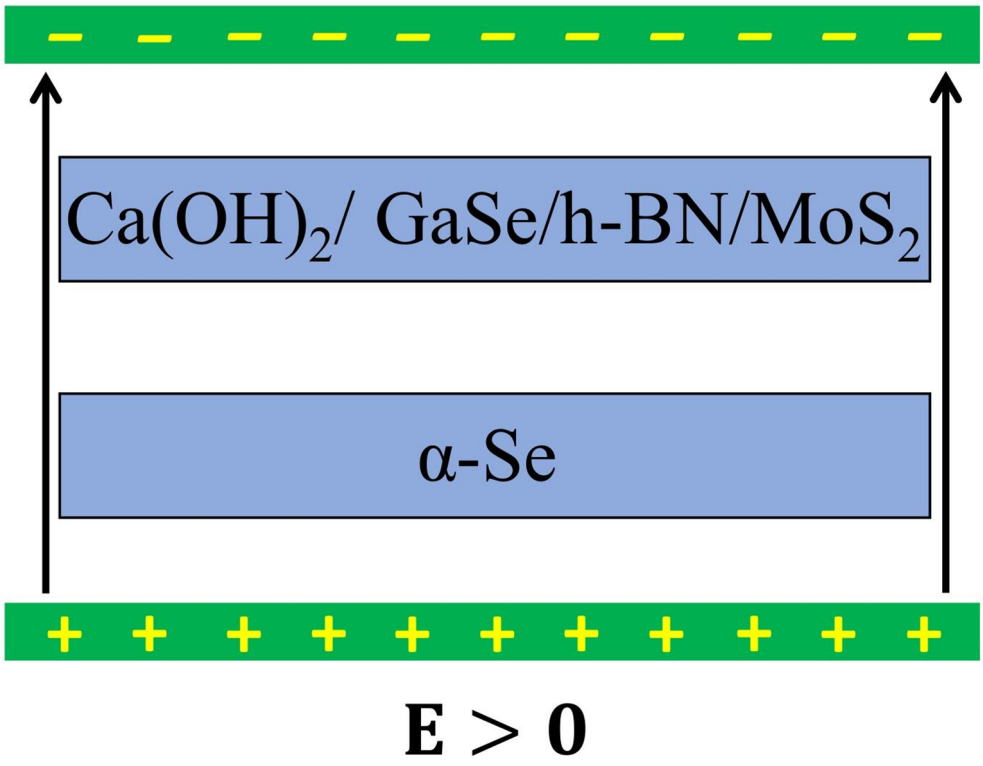

Figure S 13: (Color online). Schematic diagram of the positive electric field perpendicular to the interface of the four α-Se-based VDWHs.

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