Supplementary Material

Strain-tunable electronic structure and anisotropic transport properties in Janus MoSSe and g-SiC van der Waals heterostructure

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Calculated details of carrier mobility

The carrier mobility has been calculated in this work by the deformation potential (DP) theory via the following two formulas:

$$\mu_x = \frac{2e\hbar^3 C_x}{3K_B T m^*{}_x{}^2 E_{dx}{}^2} \tag{1}$$

$$\mu_x = \frac{e\hbar^3\left(\frac{5C_{x+}3C_y}{8}\right)}{K_B T (m_x)^{\frac{3}{2}}(m_y)^{\frac{1}{2}}\left(\frac{9E_{dx}{}^2+7E_{dx}E_{dy}+4E_{dy}{}^2}{20}\right)} \tag{2}$$

where e, $\hbar$ and K_B are electron charge, the reduced Planck constant and Boltzmann constant, T means the temperature, which is set to be 300K. C_x and E_{dx} represent the elastic modulus and deformation potential constant along the x direction (say, the armchair direction), while C_y and E_{dy} is those of along the y direction (say, the zigzag direction), respectively. C can be obtained from $C = \frac{1}{S_0}\frac{\partial^2 E}{\partial \varepsilon^2}$, where E is the total

energy of the system under uniaxial strain and S_0 is the area of the system. Here, we define the uniaxial stain as $E = (L_{strain} - L_{unstrain}) / L_{strain}$, where L_{strain} and $L_{unstrain}$ represent the lattice constants under strain and no strain respectively. E_d is represented by $E_d = \frac{\partial E_{edge}}{\partial \varepsilon}$, and E_{edge} is the energy change of band edge under uniaxial strain. At the meantime, the effective mass m^* is calculated from the following relations:

$$\frac{1}{m^*} = \frac{1}{\hbar^2} \frac{d^2 E(k)}{dk^2} \tag{3}$$

where k is wave vector and $E(k)$ represents the energy that corresponding to k.

FIGURES:

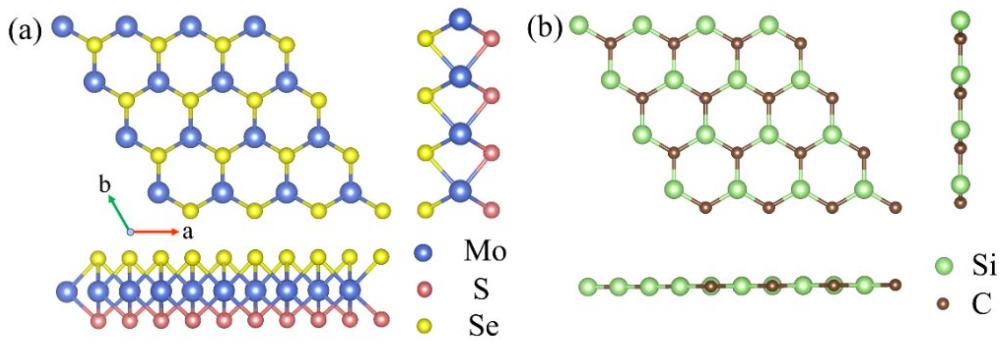

Fig. S1. The crystal structures of single-layer MoSSe and g-SiC. The blue, pink yellow, green and black balls represent the Mo, S, Se, Si and C atoms, respectively.

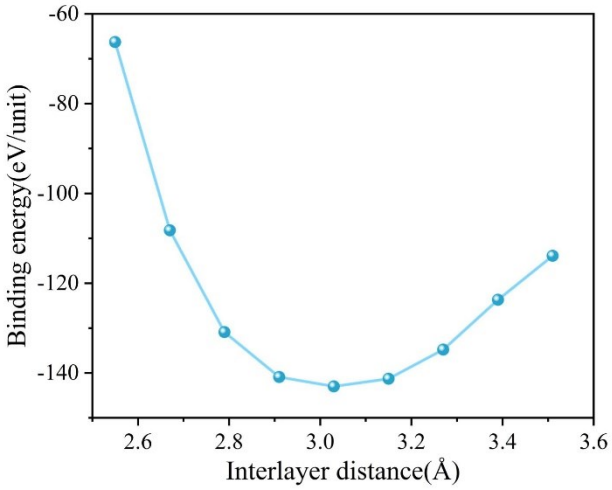

Fig. S2. The interlayer binding energy per unit cell as a function of interlayer distance for AC I-stacking.

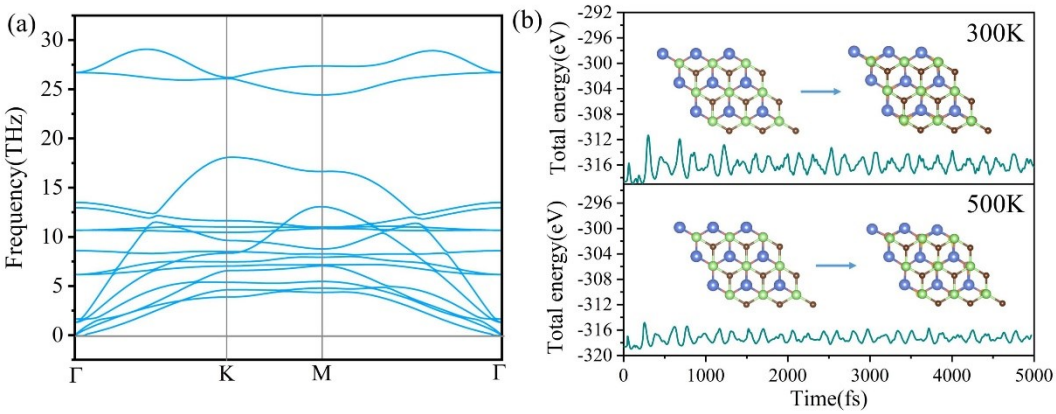

Fig. S3. (a) The phonon dispersion curve of MoSSe/g-SiC vdWH. (b) Total energy fluctuations during AIMD simulations of the MoSSe/g-SiC vdWH at 300K and 500K, where the insets show snapshots of the structures after 5 ps.

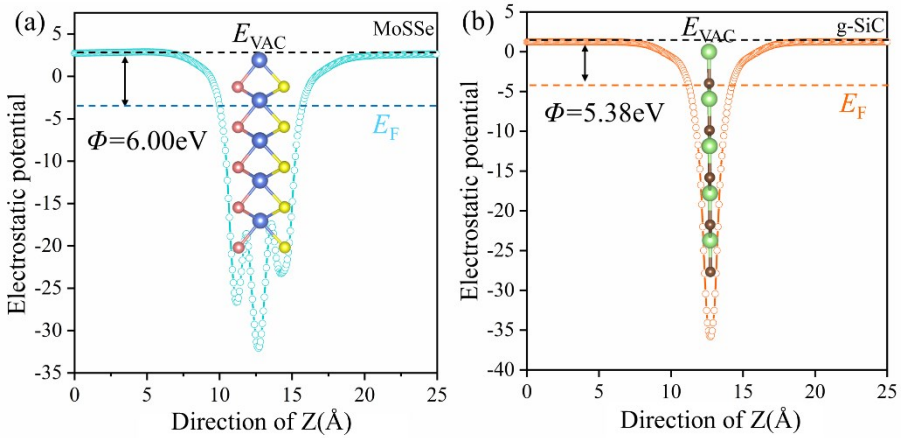

Fig. S4. The electrostatic potential of the single-layer (a) MoSSe and (b) g-SiC.

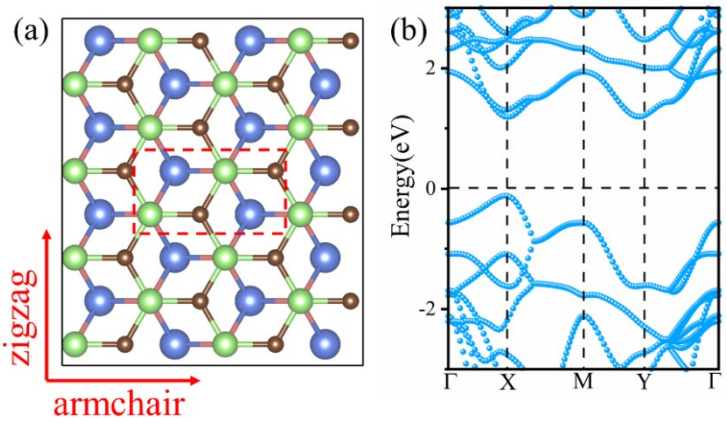

Fig. S5. (a) Top view of the atomic structure of the MoSSe/g-SiC vdWH with a rectangular supercell. The red dashed line indicates the unit cell with the zigzag and armchair directions defined. (b) Band structure of its rectangular cell calculated by the HSE06 functional.

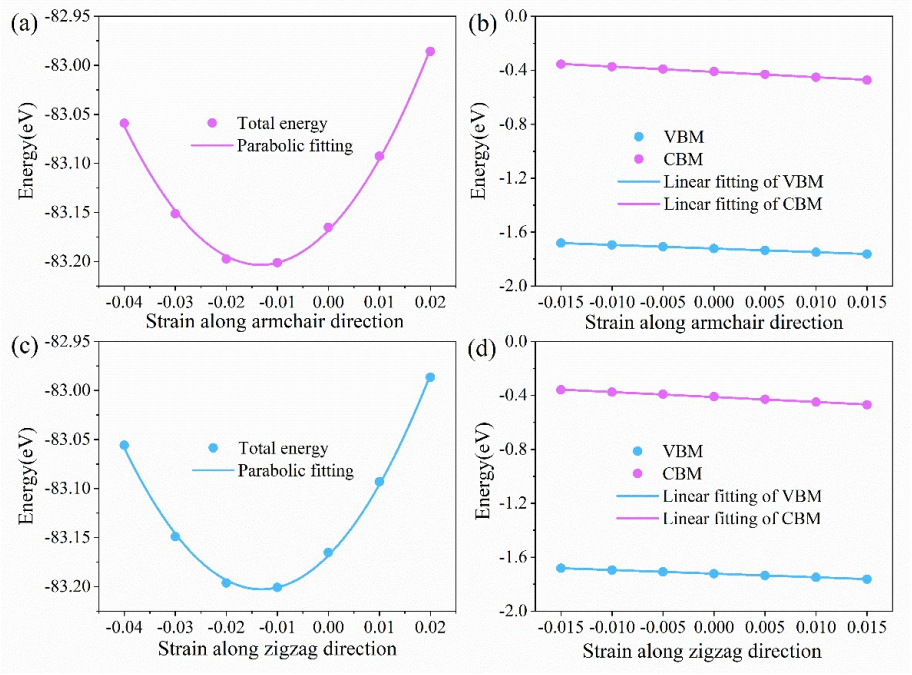

Fig. S6. The total energy (a)~(b) and energy shift of CBM and VBM (c)~(d) with respect to the lattice stretch and compression along the armchair and zigzag directions of the MoSSe/g-SiC vdWH, respectively.

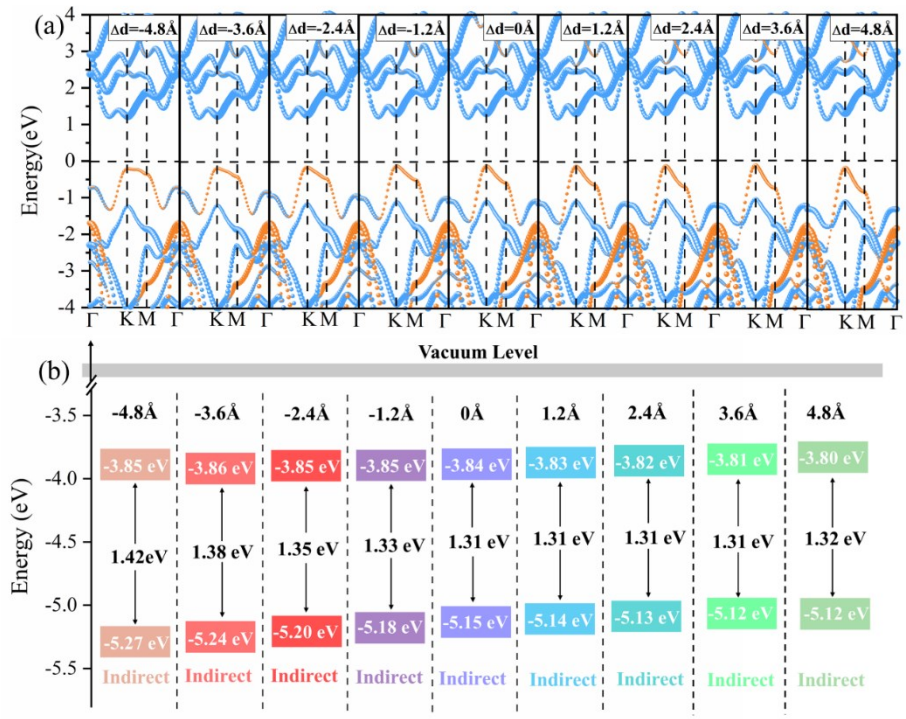

Fig. S7. (a) The band structures and (b) schematics of band alignment for MoSSe/g-SiC vdWH under various vertical strains.

Table S1 The calculated carrier mobilities of the present MoSSe/g-SiC vdWH and the previously reported heterostructure using the formula (4).

Structures	Carrier type	m^*_{arm} ($/m_0$)	m^*_{zig} ($/m_0$)	C_{arm} (N/m)	C_{zig} (N/m)	E_d^{arm} (eV)	E_d^{zig} (eV)	μ_{arm} ($cm^2/V.s$)	μ_{zig} ($cm^2/V.s$)
MoSSe/g-SiC	electron	0.60	0.60	182.63	183.30	3.94	3.68	0.46×10^3	0.53×10^3
	hole	0.57	0.57	182.63	183.30	2.70	2.70	0.10×10^4	0.11×10^4
BP/SnSe	electron	0.22	1.35	47.70	135.86	1.27	4.75	5.09×10^3	0.17×10^3
	hole	0.25	0.26	47.70	135.86	3.25	5.61	0.75×10^3	1.41×10^3
MoSSe/AlN	electron	0.64	0.64	226.92	227.03	5.54	4.53	0.38×10^3	0.58×10^3
	hole	3.91	3.28	226.92	227.03	1.11	1.11	0.28×10^3	0.33×10^3