Supplementary Information (SI) for Nanoscale.

Effect of pressure on thermoelectric performance of monolayer Janus MoSSe materials with different native vacancy defects

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Supplementary materials

Supplementary part I: Theory

Nanodcal code is based on the ballistic electronic transport theory. The transport properties is the electric current which is evaluated using the Landauer formula[1]

$$I = \frac{2e}{h}\int T_e(E)\big(f_L(E) - f_R(E)\big)dE \#(1)$$

The electrical conductivity σ, Seebeck coefficient S and thermal conductivity κ_e can be obtained from the following equations[2]

$$S = -\frac{L_1}{eTL_0} \#(2)$$

$$\sigma = \frac{e^2 L_0}{l} \#(3)$$

$$\kappa_e(T) = \frac{1}{Tl}\left(L_2 - \frac{L_1^2}{L_0}\right) \#(4)$$

where l is the device length, and $L_m(\mu)$ is given by

$$L_m(\mu) = \frac{2}{h}\int_{-\infty}^{\infty} d\varepsilon T_e(\varepsilon)(\varepsilon - \mu)^m\left(-\frac{\partial f(\varepsilon,\mu)}{\partial \varepsilon}\right) \#(5)$$

The phononic thermal conductivity can then be achieved by[2]

$$\kappa_p(T) = \frac{\hbar^2}{2\pi k_b T^2 l}\int_0^{\infty} d\omega \omega^2 T_p(\omega)\frac{e^{\frac{\hbar\omega}{k_b T}}}{\left(e^{\frac{\hbar\omega}{k_b T}} - 1\right)^2} \#(6)$$

References

1. Jeremy, T., Hong, G. & Jian, W. Ab initio modeling of quantum transport properties of molecular electronic devices. Phys. Rev. B. **63**, 245407 (2001).
2. Takahiro, Y. & Kazuyuki, W. Nonequilibrium Green's function approach to phonon transport in defective carbon nanotubes. Phys. Rev. Lett. **96**, 255503 (2006).

Supplementary part II: Figure

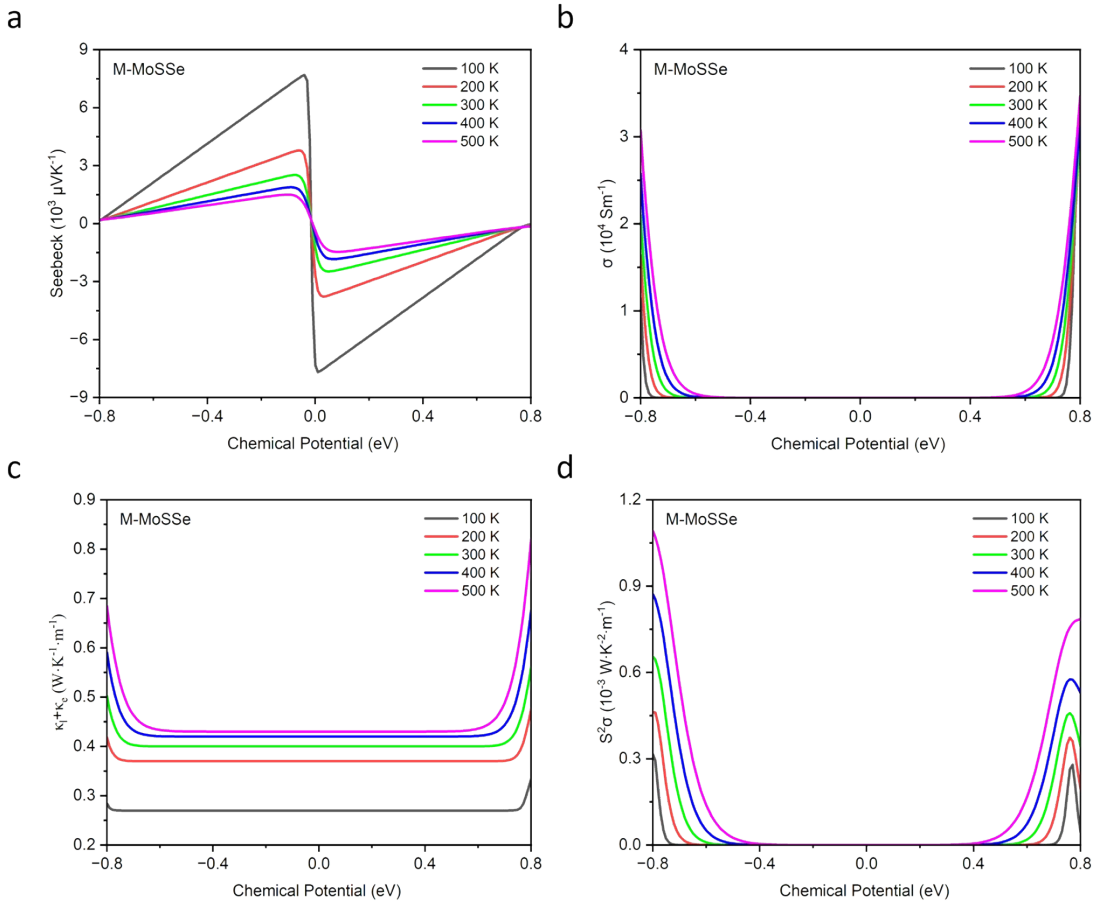

Figure .S1. Temperature dependent thermoelectric parameters as a function of chemical potential for monolayer MoSSe. (a) Seebeck coefficients. (b) conductivity. (c) electronic thermal conductivity and lattice thermal conductivity. (d) power factor.

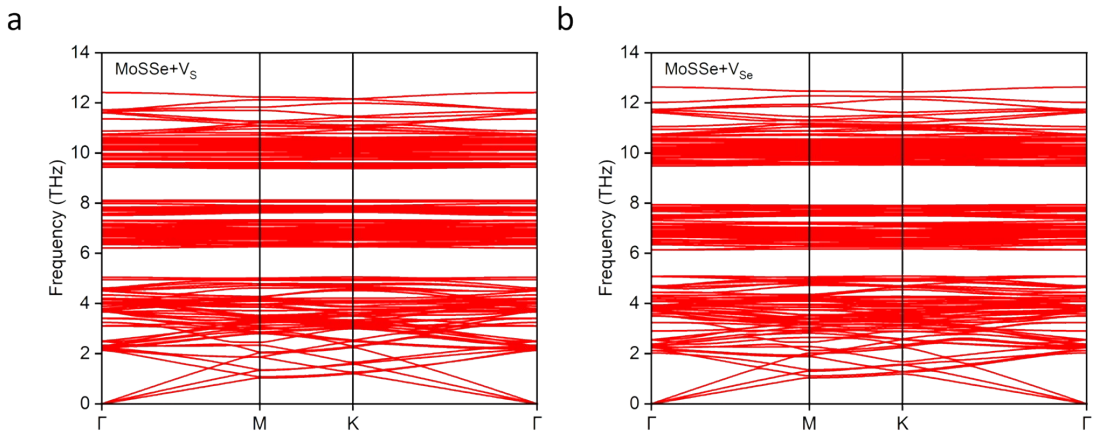

Figure .S2. phonon dispersion of (a) S defect and (b) Se defect of monolayer MoSSe.

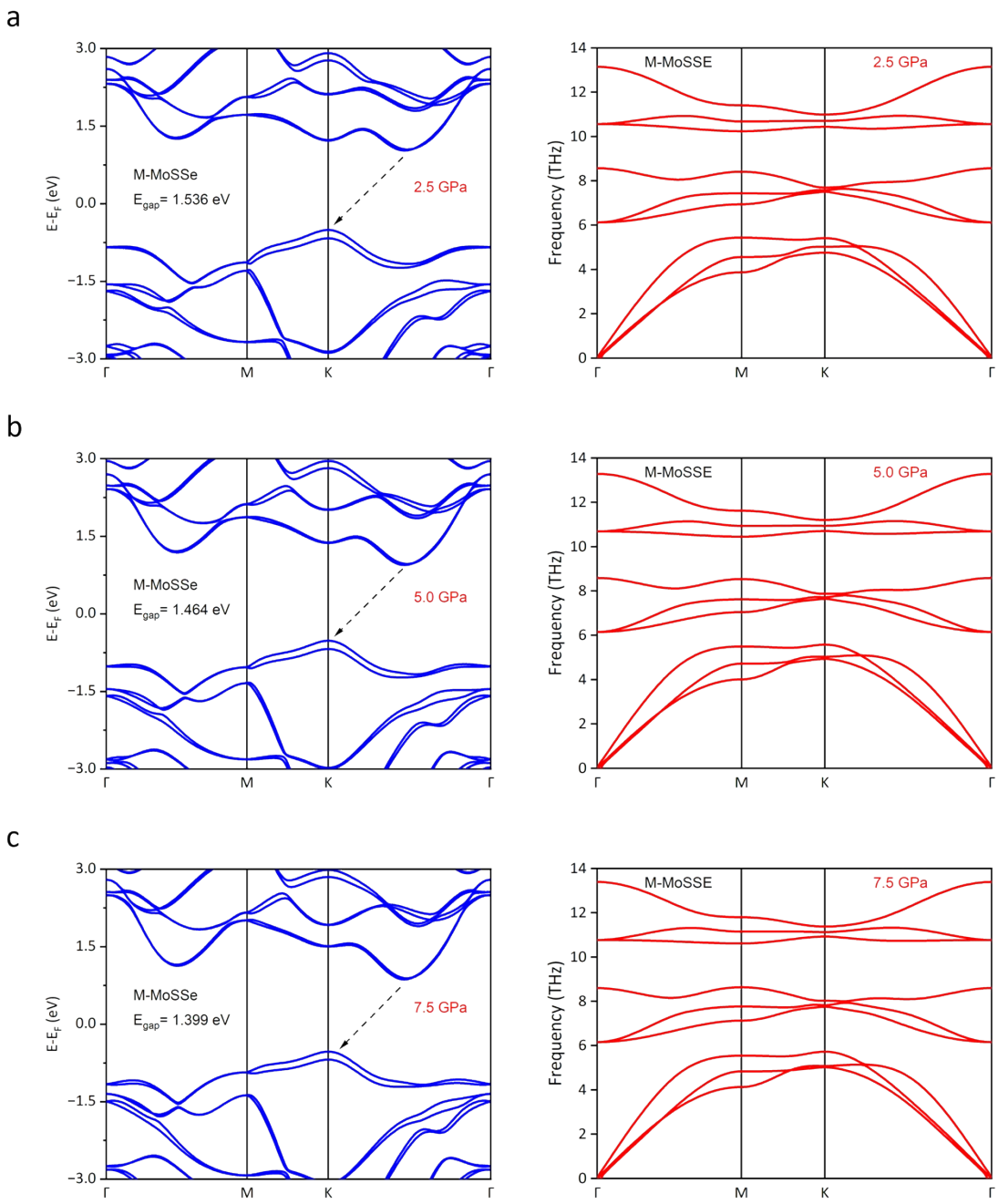

Figure .S3. Band structure and phonon dispersion. (a), (b) and (c) represent the band structure and phonon dispersion of Janus M-MoSSe under different pressure (2.5, 5 and 7.5 Gpa), respectively.

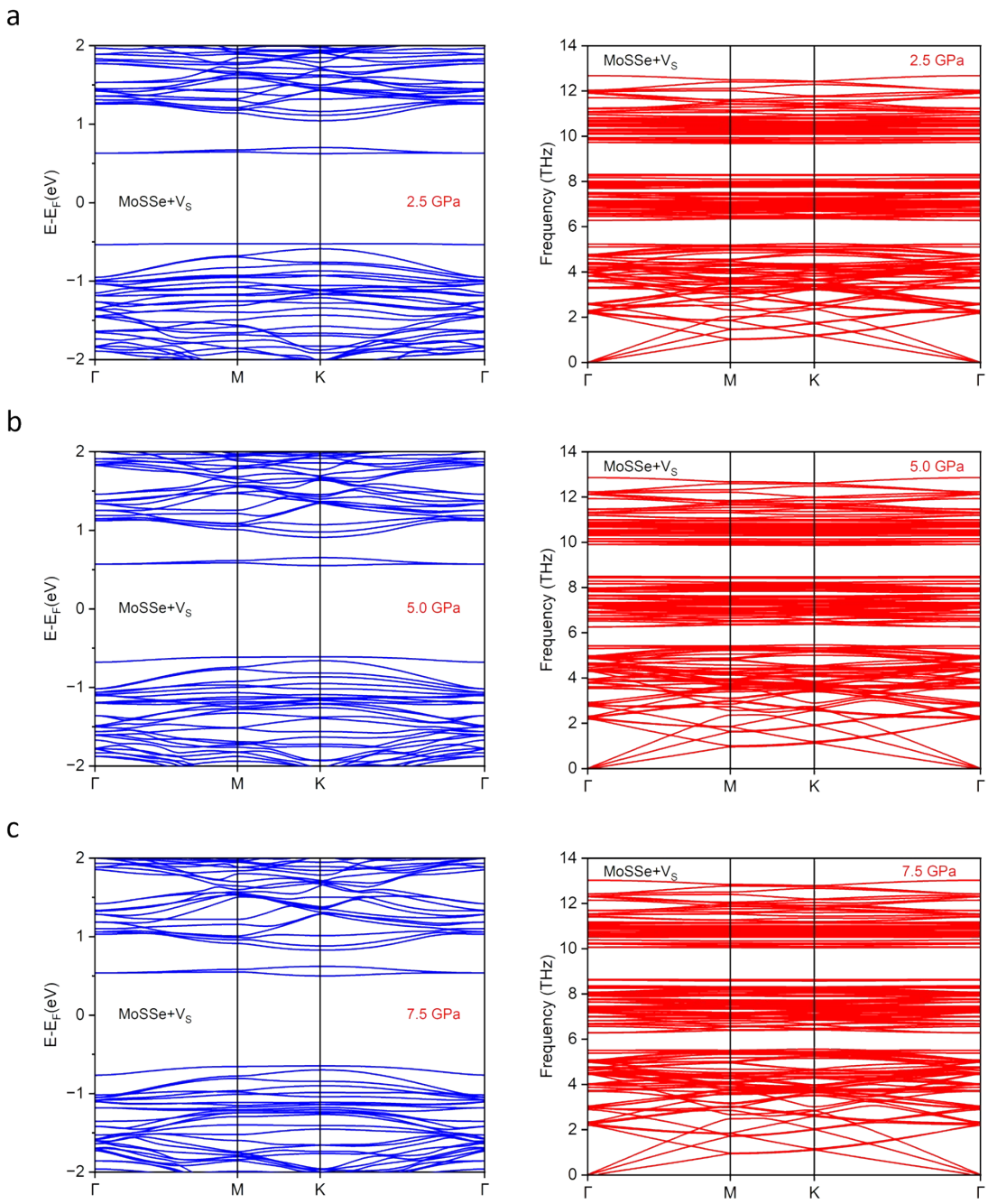

Figure .S4. Band structure and phonon dispersion. (a), (b) and (c) represent the band structure and phonon dispersion of Janus M-MoSSe with V_S vacancy defect under different pressure (2.5, 5 and 7.5 Gpa), respectively.

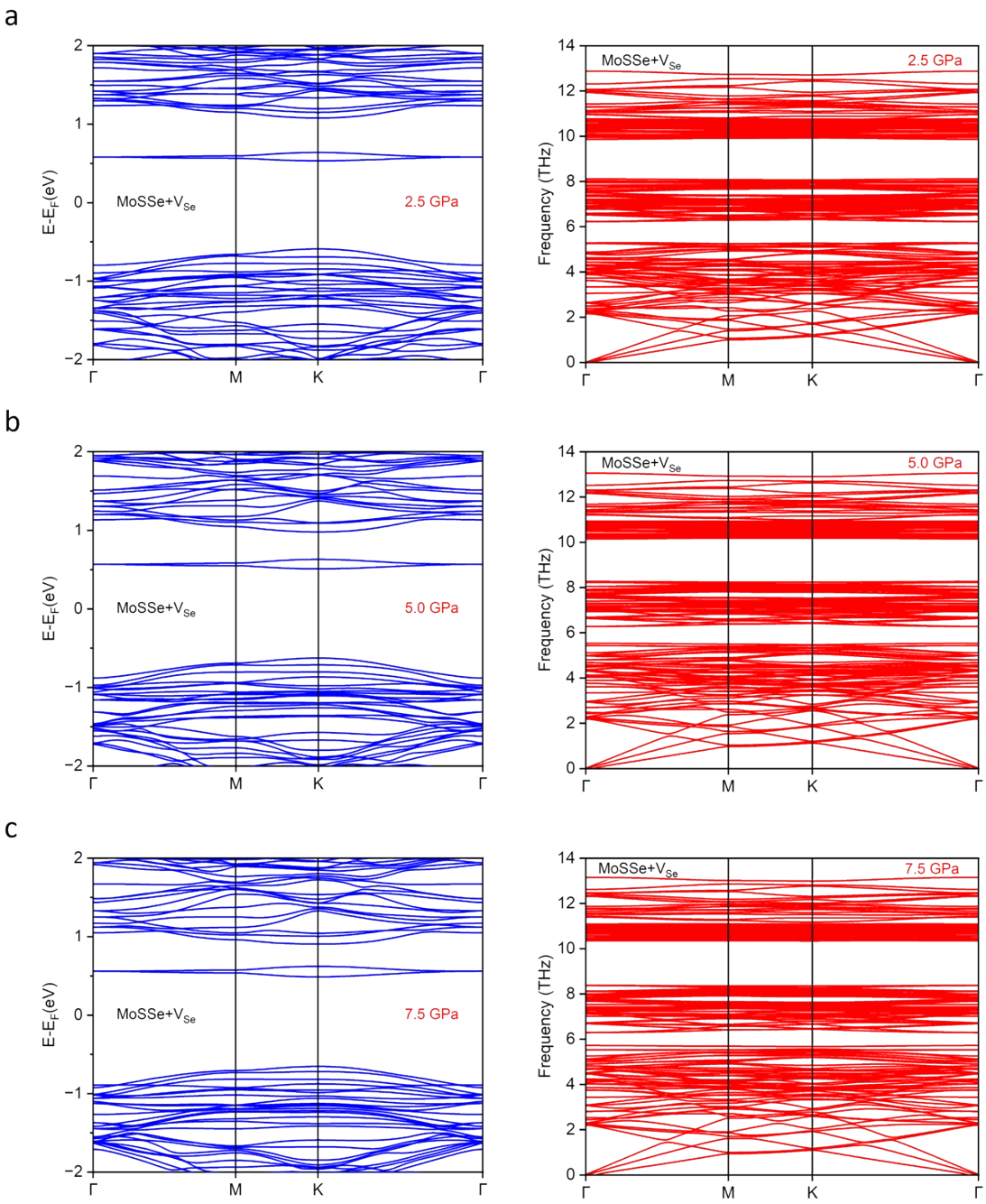

Figure .S5. Band structure and phonon dispersion. (a), (b) and (c) represent the band structure and phonon dispersion of Janus M-MoSSe with V_{Se} vacancy defect under different pressure (2.5, 5 and 7.5 Gpa), respectively.