

Supplementary Information

for

SnSe₂ monolayer with square lattice structure: A promising *p*-type thermoelectric material with indirect bandgap and low lattice thermal conductivity

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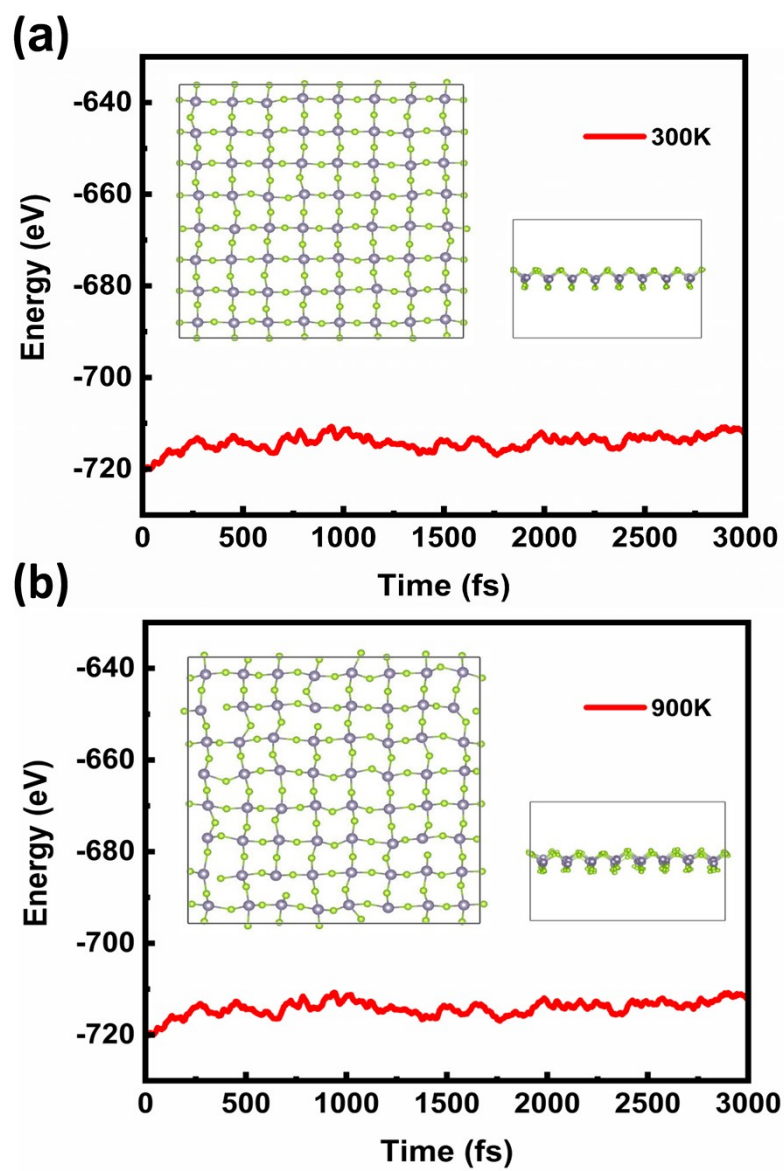


Figure. S1. The snapshots of AIMD simulations of the SnSe₂ monolayer at (a) 300K and (b) 900K. The black and green balls represent the Sn and Se atoms, respectively.

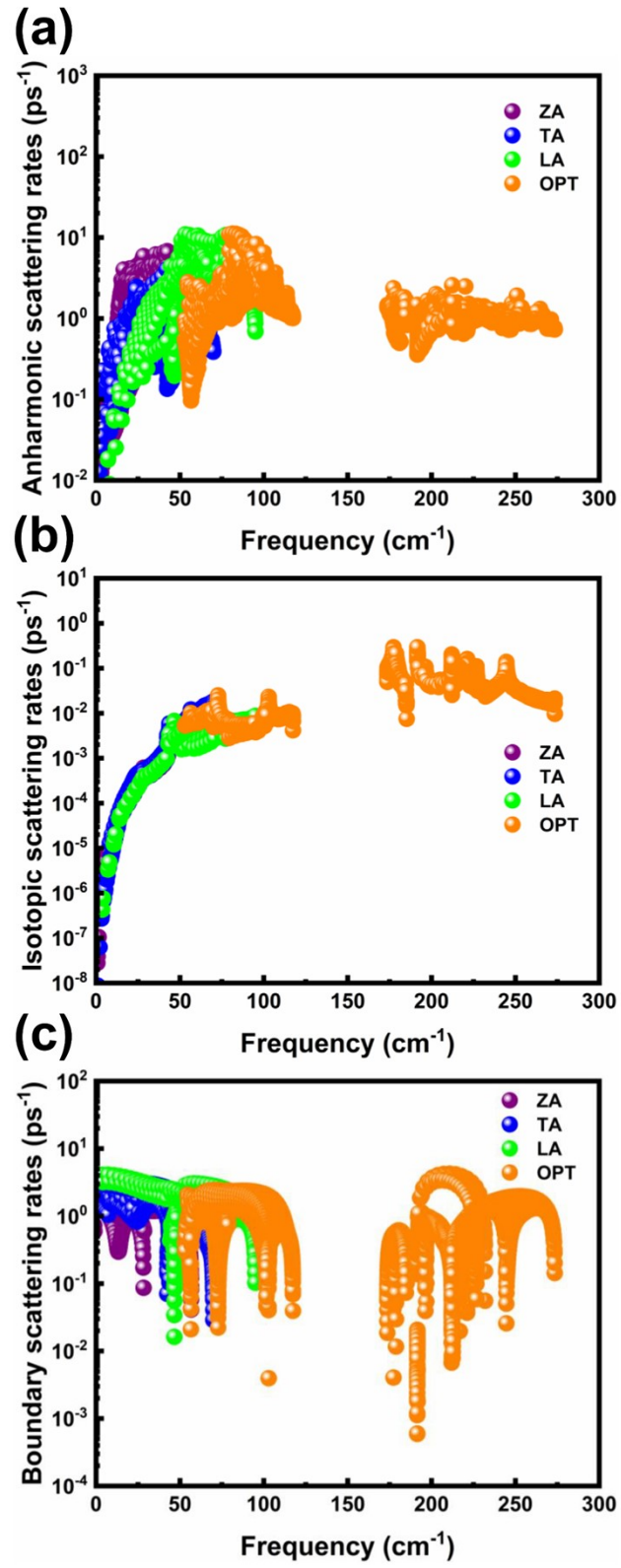


Figure.S2. (a) Anharmonic scattering rates, (b) Isotopic scattering rates, and (c) Boundary scattering rates of SnSe₂ monolayer.

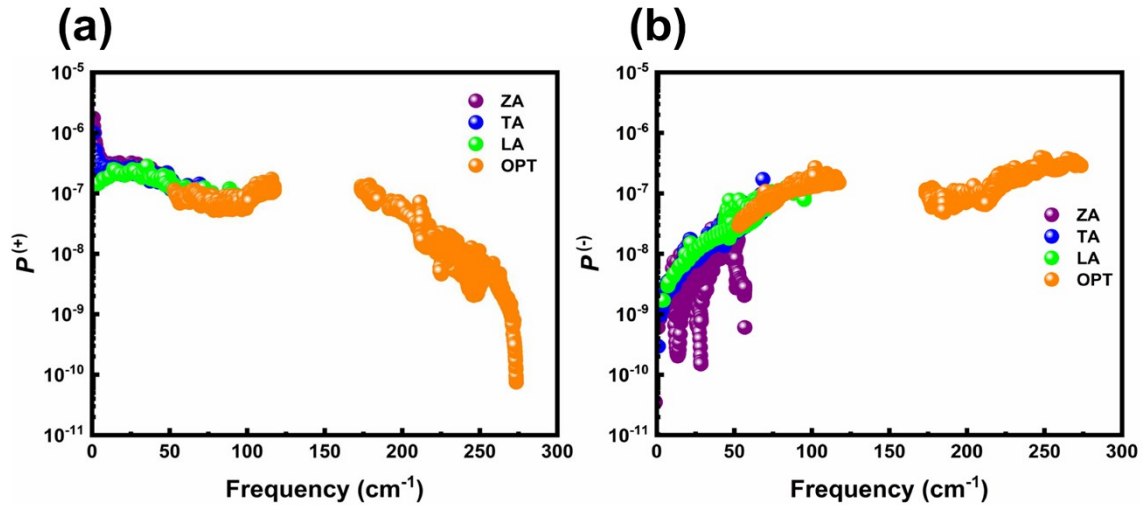


Figure S3. Phase spaces for (a) absorption and (b) emission processes of SnSe₂ monolayer.

Table S1. The carrier mobility (μ , $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$) and relaxation time (τ , ps) for electrons and holes of SnSe_2 monolayer at 300, 500, 700 and 900K.

Temperature	Carriers	μ_{2D} ($\text{cm}^2/\text{V}\cdot\text{s}$)	τ (ps)
300K	hole	71.28	0.063
	electron	115.39	0.053
500K	hole	42.77	0.038
	electron	69.24	0.032
700K	hole	30.55	0.027
	electron	49.45	0.023
900K	hole	23.76	0.021
	electron	38.46	0.018