Supporting information

Thermoelectric performance of Janus monolayer embedded in MX_2-based superlattice: A computational insight

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Debye temperature calculation

The Debye temperature θ_D can be calculated from the average group velocity as v_a,

$$\theta_D = \frac{\hbar v_a}{k_B}\left(\frac{4\pi N}{s}\right)^{1/2} \quad (1)$$

Where, $\hbar$ is the reduced Planck's constant, k_B is the Boltzmann constant, N is the number of atoms in the unit cell, S is the area of the unit cell, and v_a is the average group velocity given by,

$$v_a = \left[\frac{1}{3}\left(\frac{1}{v_l^3} + \frac{2}{v_t^3}\right)\right]^{-1/3} \quad (2)$$

Table S1. Calculated values of deformation potential constant (E_1), elastic constant (C_{3D}), carrier effective mass (m^*) and longitudinal acoustic-phonon limited mobility (μ_{LA}) are calculated at 300K. m_0 : bare electron mass (9.1×10^{-31} Kg).

Materials		E_1 (eV)	C_{3D}x10^{10} (j/m^3)	$m^*(m_0)$	Mobility (μ_{LA}) (cm^2/Vs)
$HfSe_2$/HfSSe/$HfTe_2$	**electrons**	2.22	0.99	0.212	5608
	holes	3.37		0.170	4226
$HfSe_2$/HfSeTe/$HfTe_2$	**electrons**	1.47	0.60	0.30	3254
	holes	6.98		0.20	397
$HfSe_2$/HfSTe/$HfTe_2$	**electrons**	1.61	5.82	0.18	9368
	holes	7.26		0.12	12788

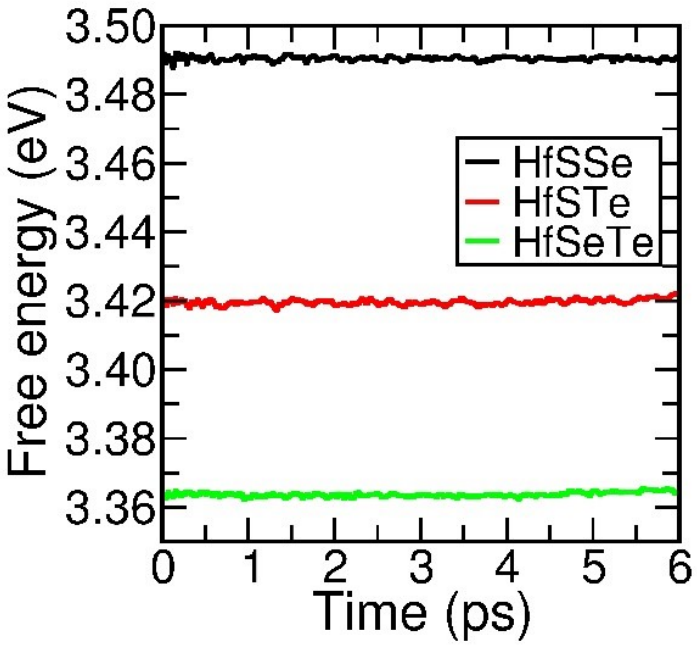
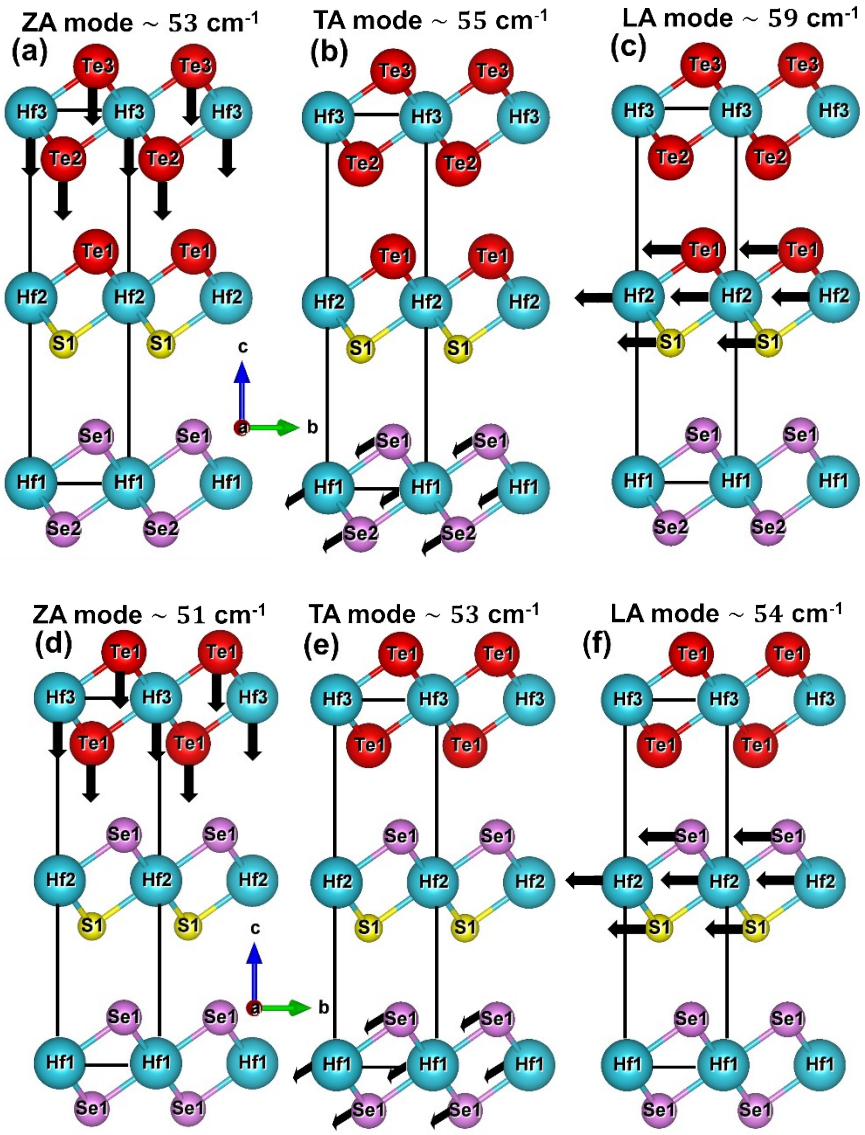


Figure S1. Time evolution of free energy up to 6 ps during AIMD simulations for all three superlattices at 700 K.


ZA mode ~ 53 cm-1
(a)
TA mode ~ 55 cm-1
(b)
LA mode ~ 59 cm-1
(c)
ZA mode ~ 51 cm-1
(d)
TA mode ~ 53 cm-1
(e)
LA mode ~ 54 cm-1
(f)
Te3
Te2
Te1
Hf3
Hf2
Hf1
S1
Se1
Se2
c
b

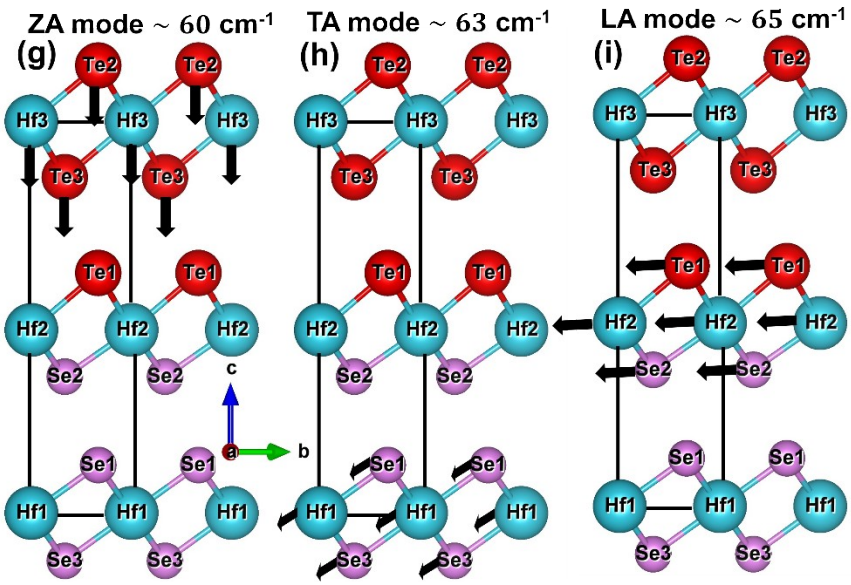


Figure S2. The The observed eigen vectors at K point for Janus SL (a) HfSTe, (b) HfSSe and (c) HfSeTe mode. Here the black arrow represents the direction of the mode of vibration. LA mode involves atomic displacements along the direction of wave propagation, the TA mode involves atomic displacements perpendicular to the propagation direction and the ZA mode involves out of-plane vibrations.

Table S2. The calculated lattice thermal conductivity (κ_{latt}) and Seebeck coefficient of all three Janus SL for temperature range of 300 to 700K.

Temp.	HfSSe			HfSTe			HfSeTe		
	S_e (μV/K)	S_h (μV/K)	κ_{latt} (W/mK)	S_e (μV/K)	S_h (μV/K)	κ_{latt} (W/mK)	S_e (μV/K)	S_h (μV/K)	κ_{latt} (W/mK)
300	1821	2006	0.80	2126	2438	0.65	1885	2177	1.1
400	1325	1527	0.60	1503	1836	0.48	1363	1674	0.9
500	1035	1255	0.50	1135	1499	0.39	1040	1370	0.72
600	836	1073	0.42	900	1274	0.33	822	1180	0.60
700	696	916	0.36	716	1090	0.28	660	1028	0.51

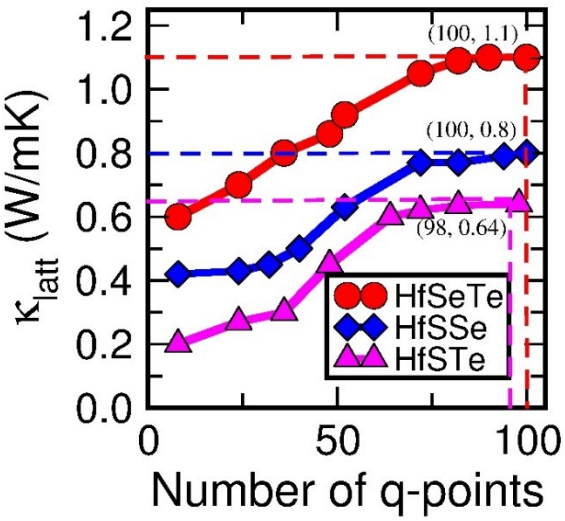


Figure S3. Lattice thermal conductivity convergence test for all three SL systems.

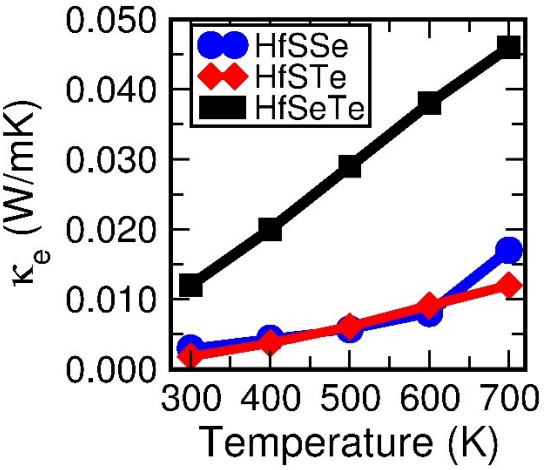


Figure S4. The calculated electronic component of thermal conductivity (κ_e) for all the superlattices.

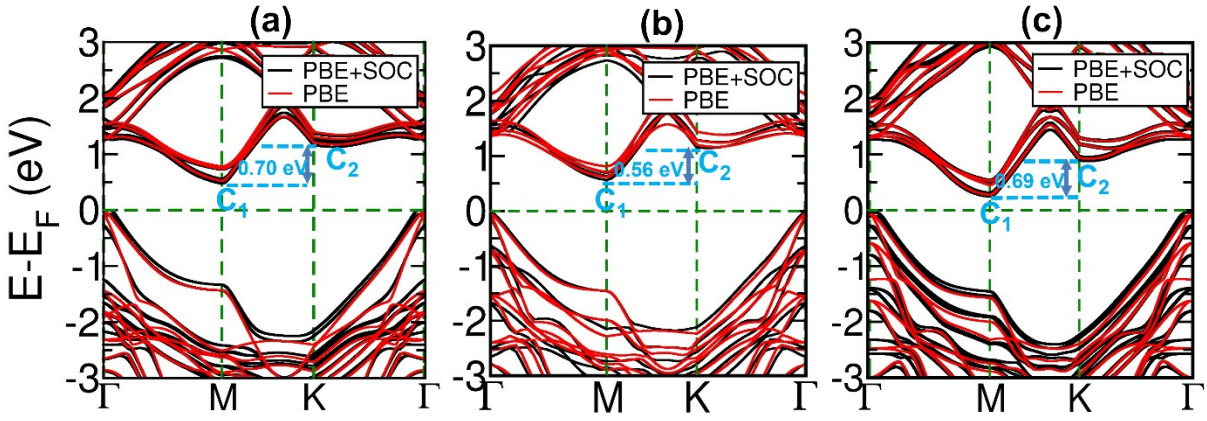


Figure S5. Comparison of the electronic band structures with and without spin–orbit coupling (SOC) for (a) HfSSe, (b) HfSTe and (c)HfSeTe SL.

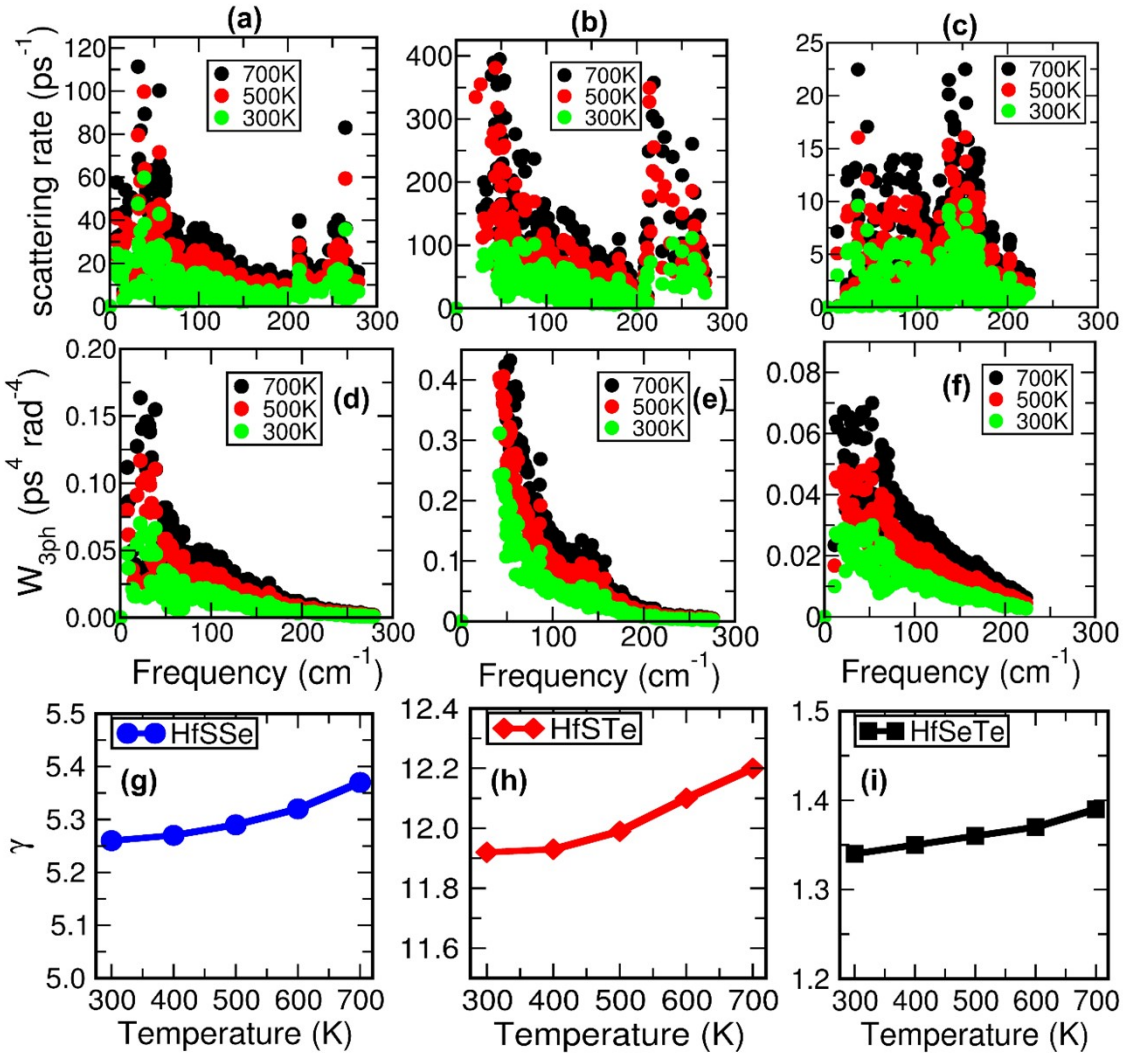


Figure S6. Computed scattering rate, Grüneisen parameter and phase space for $HfSe_2$/HfSSe/$HfTe_2$ (a), (d), (g), $HfSe_2$/HfSTe/$HfTe_2$ (b), (e), (h) and $HfSe_2$/HfSeTe/$HfTe_2$ (c), (f), (i) at high temperatures.

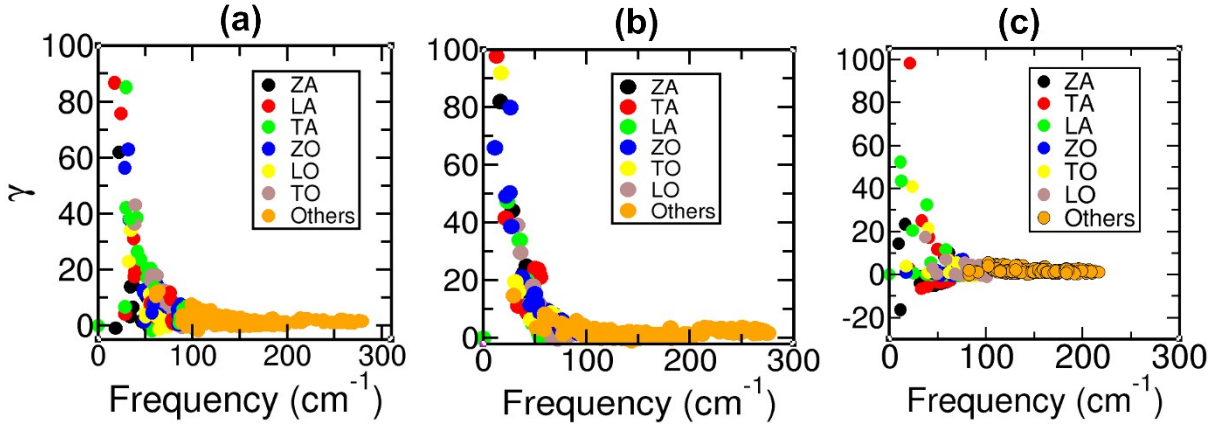


Figure S7. Calculated mode resolved Grüneisen parameter for (a) HfSSe, (b) HfSTe and (c) HfSeTe system.