Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Unravelling Hidden Mechanisms in Heterostructure and Superlattice Beneficial for Thermoelectricity

Tanu Choudhary[1], Satarupa Banik[1], Jipin Peter[1], Raju K Biswas[1,2,*]

[1]Department of Physics, Faculty of Natural Sciences,

M S Ramaiah University of Applied Sciences, Bengaluru 560058, India

[2]Department of Physics, North Eastern Regional Institute of Science and Technology, Nirjuli, Arunanchal Pradesh, 791109, India

E-mail: rkb@nerist.ac.in

Supporting Information

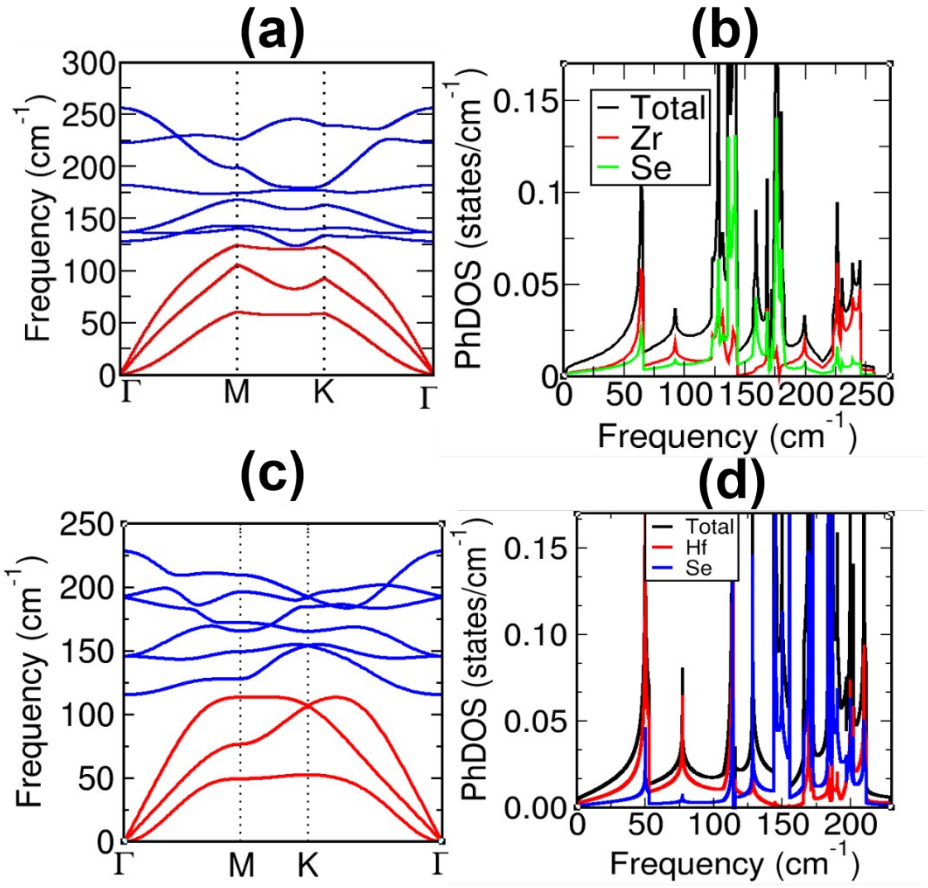

Fig. S1. Phonon bands dispersion and phonon DOS for (a),(b) $ZrSe_2$ and (c),(d) $HfSe_2$ along the high symmetry points *Γ– M – K – Γ* in the Brillouin zone.

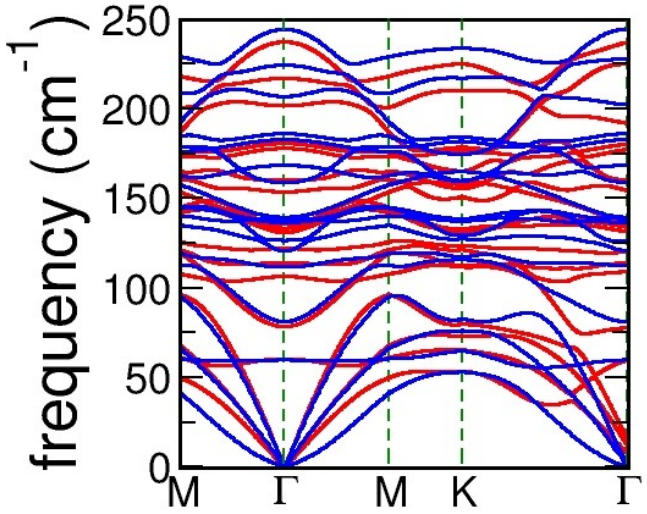

Fig. S2. Phonon bands dispersion for SLM at 1% strain with comparison in 0% strain along the high symmetry points *M– Γ– M – K– Γ* in the Brillouin zone. Here red colour bands show the strain dispersion and blue referees to unstrained system.

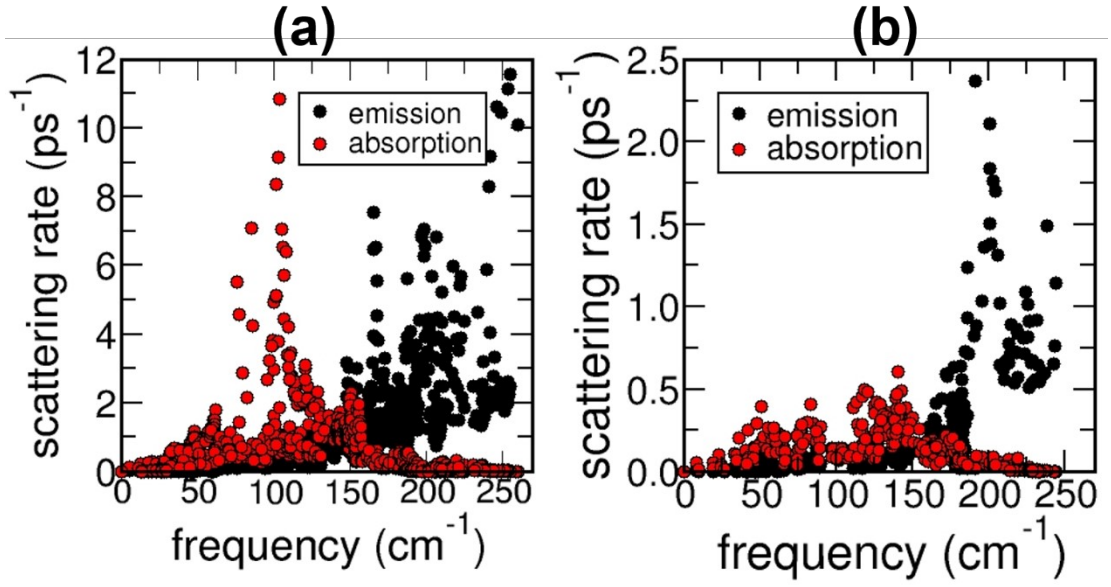

Fig. S3. Calculated decomposed emission and absorption scattering rate as a function of frequency for (a) HS and (b) SLM, respectively.

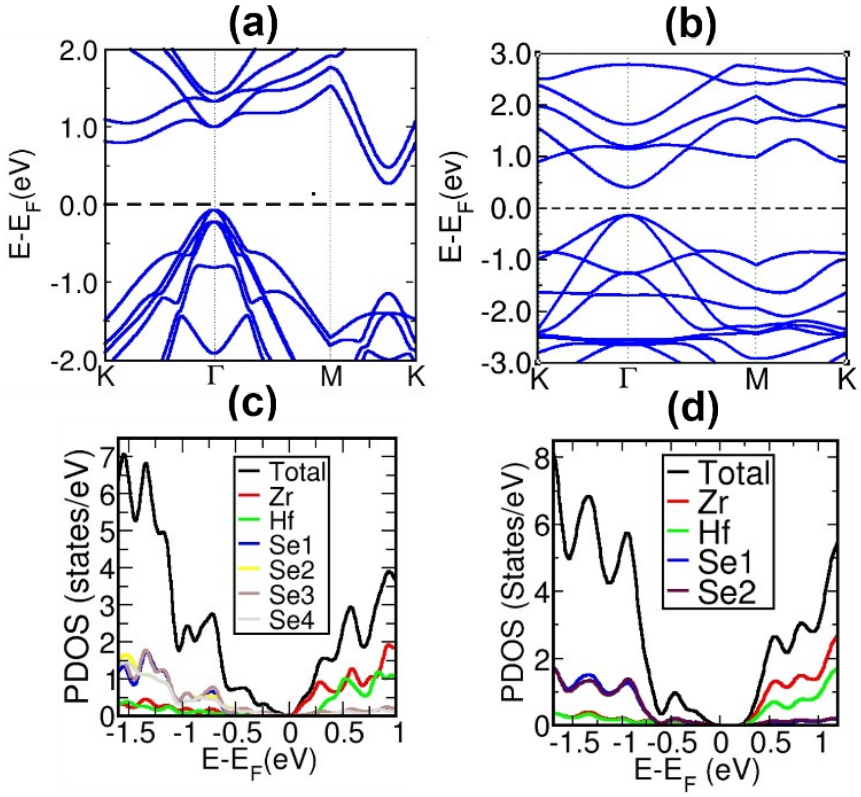

Fig. S4. The electronic band structure and projected DOS of (a),(c) HS and (b),(d) SLM. The band gap is represented by the arrow

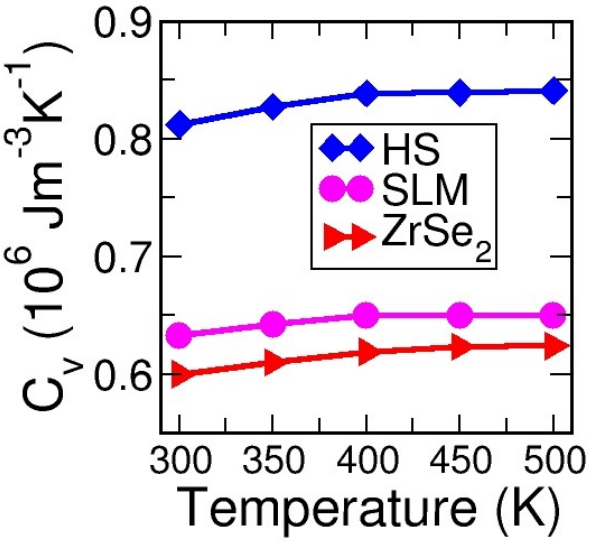

Fig. S5. The calculated specific heat of $ZrSe_2$, HS and SLM.

Table S1. The calculated hole mobility (μ_h), electron mobility (μ_e) and *n*- and *p*-type Seebeck coefficient (*S*) of HS and SLM for temperature range of 300 to 500K.

Temperature (K)	HS				SLM			
	μ_h [$cm^2v^{-1}s^{-1}$]	μ_e [$cm^2v^{-1}s^{-1}$]	S_n (μV/K)	S_p (μV/K)	μ_h [$cm^2v^{-1}s^{-1}$]	μ_e [$cm^2v^{-1}s^{-1}$]	S_n (μV/K)	S_p (μV/K)
300	6319	3610	839	887	375	306	192	227
350	5653	3093	980	1037	324	282	235	263
400	4739	2707	1119	1183	281	229	260	302
450	4396	2406	1271	1343	252	220	299	338
500	3791	2166	1401	1478	225	183	329	379

Table S2. The calculated electronic part of thermal conductivity (κ_e) of HS and SLM for temperature range of 300 to 500K.

	κ_e(W/mK) SLM		κ_e(W/mK) Bilayer HS	
Temperature	**n-type**	**p-type**	**n-type**	**p-type**
300	3.72×10^{-4}	4.5×10^{-4}	4.1×10^{-5}	7.4×10^{-5}
350	6.8×10^{-4}	7.8×10^{-4}	7.2×10^{-5}	1.3×10^{-4}
400	9.2×10^{-4}	1.1×10^{-3}	1.0×10^{-4}	1.8×10^{-4}
450	1.34×10^{-3}	1.5×10^{-3}	1.4×10^{-4}	2.5×10^{-4}
500	1.70×10^{-3}	1.9×10^{-3}	1.7×10^{-4}	3.1×10^{-4}

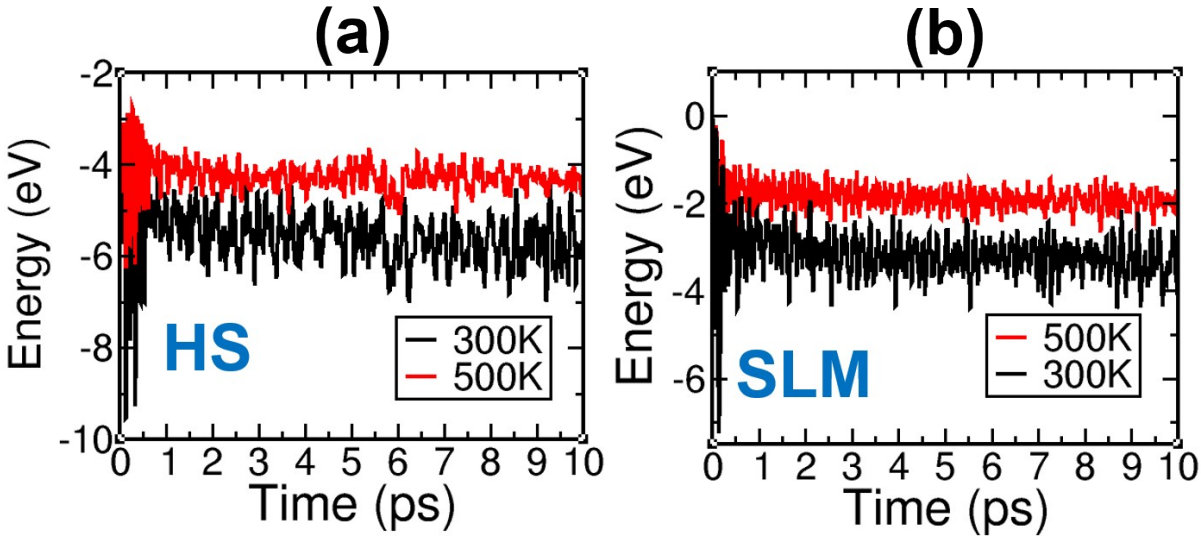

Fig. S6. Time evolution of total energy up to 10 ps during AIMD simulations for (a) bilayer HS and (b) SLM at 300 K and 500 K.