Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

SUPPORTING INFORMATION

Systems	Temperature (K)	Mobility ($cm^2 V^{-1} s^{-1}$)	
		p – type	n – type

Emergence of promising n – type thermoelectric material through conductive network and strong phonon softening

Jipin P M,[1] Tanu Choudhary,[1] Raju K Biswas *,[1]

[1]*Department of Physics, Faculty of Mathematical and Physical Sciences*

M S Ramaiah University of Applied Sciences,

*Bengaluru 560058, India, *rajukumar1718@gmail.com*

Table S1. Calculated lattice parameters (a=b), bond length (d), bond angle and band gap of $HfSe_2$, Janus HfSeS and $HfSeS_{0.5}Te_{0.5}$ monolayers.

Systems	Lattice constant, a=b (Å)	Bond length, d (Å)	Bond angle (Degree)	Band gap (eV)
$HfSe_2$	3.76 [24,51]	2.68 (Hf – Se) [24,51]	81.45° (Hf – Se – Hf)	0.67 [24,52]
HfSeS	3.70	2.68 (Hf – Se) 2.54 (Hf – S)	87.45° (Hf – Se – Hf) 93.24° (Hf – S – Hf)	0.88
$HfSeS_{0.5}Te_{0.5}$	7.62	2.68 (Hf – Se) 2.57 (Hf – S) 2.90 (Hf – Te)	88.01° (Hf – Se – Hf) 93.19° (Hf – S – Hf) 83.78° (Hf – Te – Hf)	0.11

Systems	Temperature (K)	Seebeck coefficient (μV/K)	
		p-type	n-type
$HfSe_2$	300	1252.50	395.87
	450	835.00	263.91
	600	626.25	197.93
	750	501.00	158.34
	900	417.50	131.95
	1050	357.85	113.10
	1200	313.12	98.96
HfSeS	300	4319.02	894.70
	450	2878.68	596.47
	600	2159.01	447.35
	750	1727.20	357.88
	900	1439.34	298.23
	1050	1233.72	255.63
	1200	1079.50	223.67
$HfSe_2$	300	8973.83	3054.65
	450	5982.56	2023.10
	600	4486.91	1517.32
	750	3589.53	1213.86
	900	2991.28	1011.55
	1050	2563.95	867.04
	1200	2243.45	758.66
$HfSeS_{0.5}Te_{0.5}$	300	1690	407
	450	1127	271
	600	845	203
	750	676	163
	900	563	136
	1050	483	116
	1200	422	102

Table S2. Calculated carrier mobility for p and n – type $HfSe_2$, Janus HfSeS and $HfSeS_{0.5}Te_{0.5}$ monolayers at different temperatures.

Systems	Temperature (K)	κ_l (W/mK)		
	300	1386		1372
	450	921		894
	600	681		647
HfSeS	750	539		496
	900	440		403
	1050	372	1.65	336
	1200	324	1.29	280
	600		1.03	
	750		0.85	
$HfSe_2$	300	2773		2920
	900		0.72	
	450	2058		2016
	1050		0.62	
	600	1596		1554
	1200		0.54	
$HfSeS_{0.5}Te_{0.5}$	750	1302		1260
	900	1120		1078
	300		1.92	
	1050	973		959
	450		1.58	
	1200	876		850
	600		1.29	
HfSeS	750		1.07	
	900		0.91	
	1050		0.79	
	1200		0.69	
	300		1.07	
	450		0.87	
	600		0.70	
$HfSeS_{0.5}Te_{0.5}$	750		0.58	
	900		0.49	

Table S3. Calculated Seebeck coefficient values of p and n – type $HfSe_2$, Janus HfSeS and $HfSeS_{0.5}Te_{0.5}$ monolayers at different temperatures.

	1050	0.42
	1200	0.37

Table S4. Calculated lattice thermal conductivity (κ_l) values for $HfSe_2$, Janus HfSeS and $HfSeS_{0.5}Te_{0.5}$ monolayers at different temperatures.

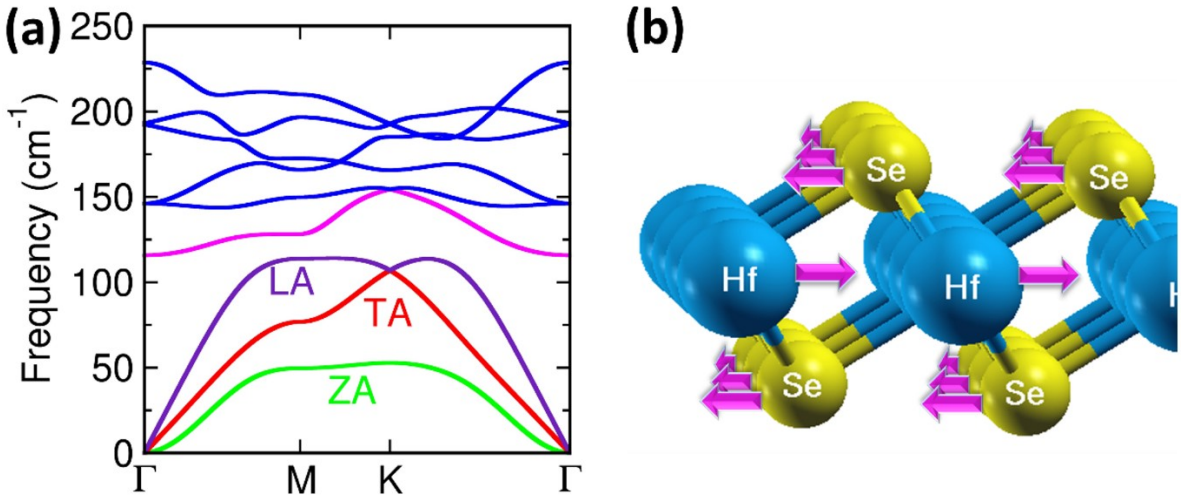

Fig. S1 (a) Phonon dispersion bands along $\Gamma - M - K - \Gamma$ direction in the Brillouin zone and (b) Eigen vectors for $HfSe_2$ monolayer.

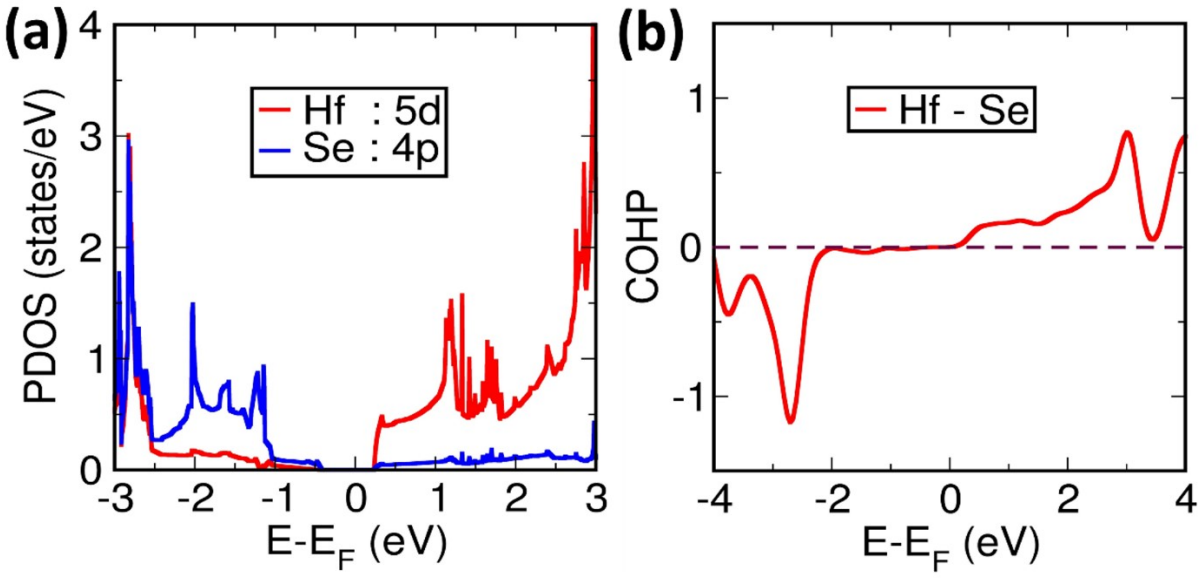

Fig. S2 (a) Projected density of states and (b) crystal orbital Hamilton population (COHP) plot as a function of energy (E) for $HfSe_2$ monolayer.

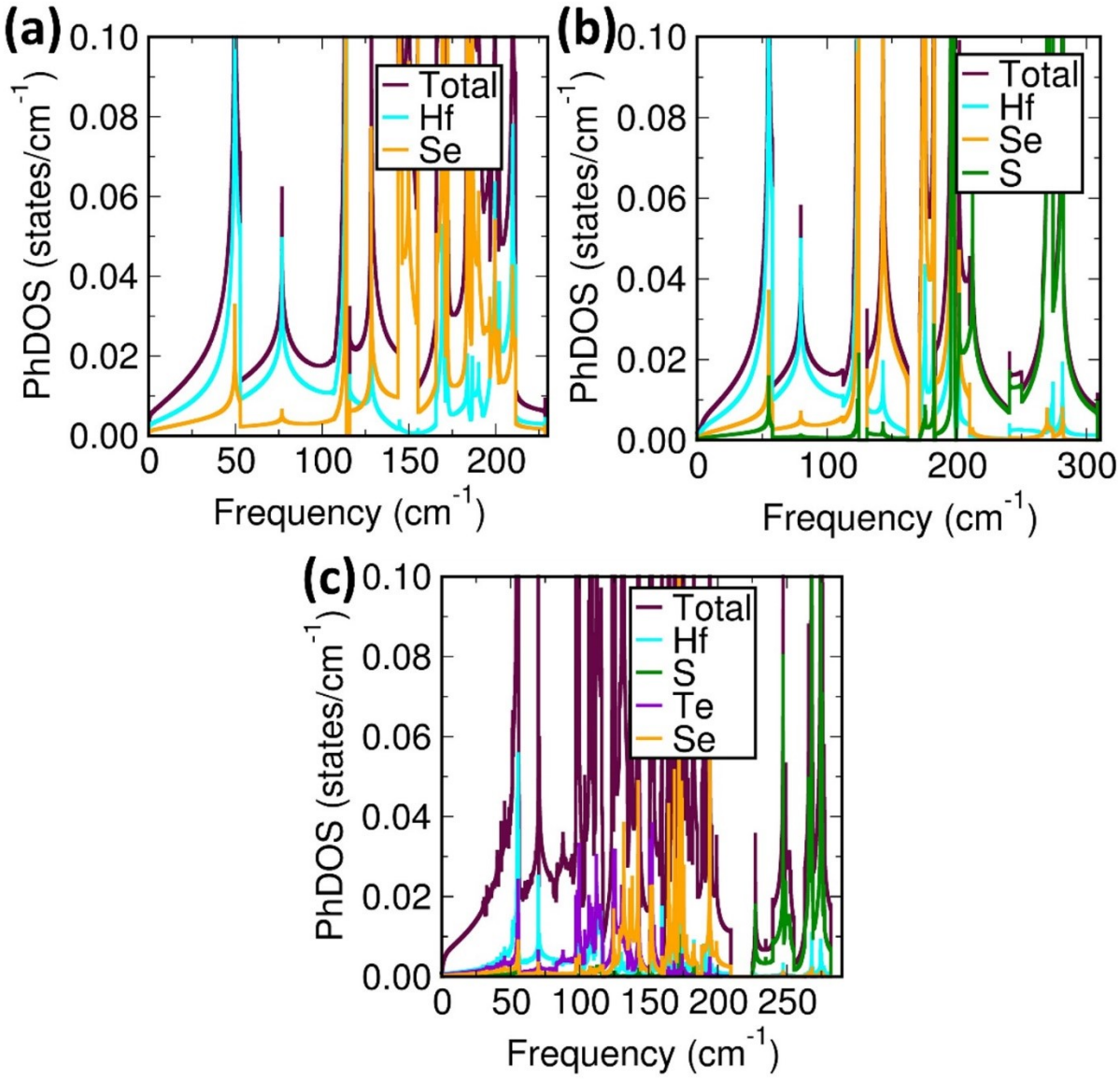

Fig. S3 Phonon density of states for (a) $HfSe_2$, (b) Janus HfSeS and (c) $HfSeS_{0.5}Te_{0.5}$ monolayers, respectively.

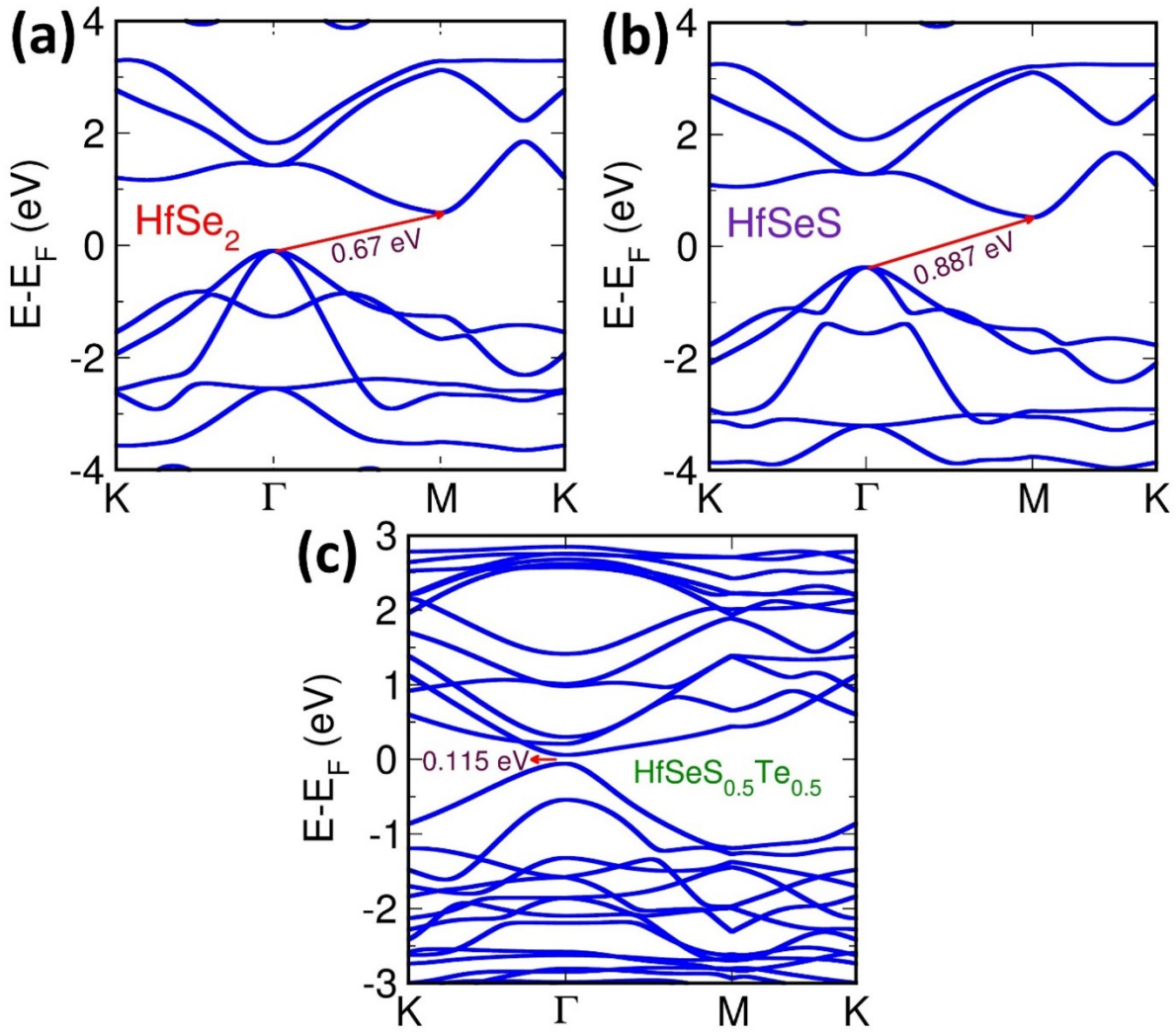

Fig. S4 Electronic band structure calculated along the high symmetry points $K-\Gamma-M-K$ using density functional theory (DFT) within PBE functional for (a) $HfSe_2$, (b) Janus HfSeS and (c) $HfSeS_{0.5}Te_{0.5}$ monolayers, respectively.

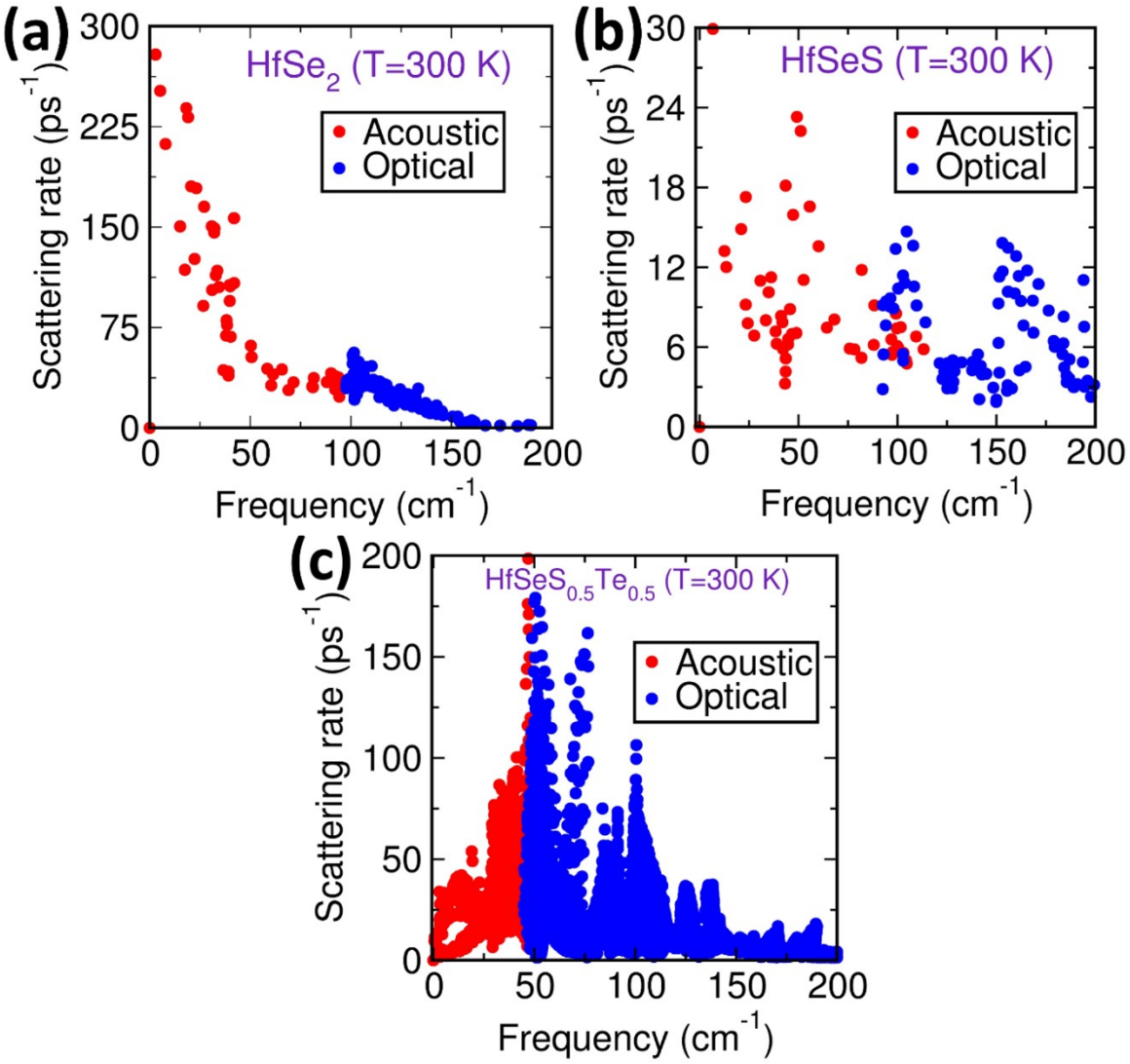

Fig. S5 Phonon scattering rate as a function of phonon frequency for (a) $HfSe_2$, (b) Janus HfSeS and (c) $HfSeS_{0.5}Te_{0.5}$ monolayers, respectively at 300 K. Red and blue colour corresponds to acoustic and optical phonons, respectively.