Supplementary Material: Effect of Electron-Phonon Coupling on Transport Properties of Monolayers of ZrS_2, BiI_3 and PbI_2: A thermoelectric Perspective

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TABLE S1. Pauling electronegativity (EN) values for the different elements present in the monolayers.[1] Difference between the electronegativity (ΔEN) of the elements present in the monolayers.

Element	EN
Zr	1.33
Pb	2.33
Bi	2.02
I	2.66
S	2.58
System	ΔEN
ZrS_2	1.25
BiI_3	0.64
PbI_2	0.33

I. MODE-RESOLVED IMAGINARY PART OF ELECTRON-PHONON SELF-ENERGY

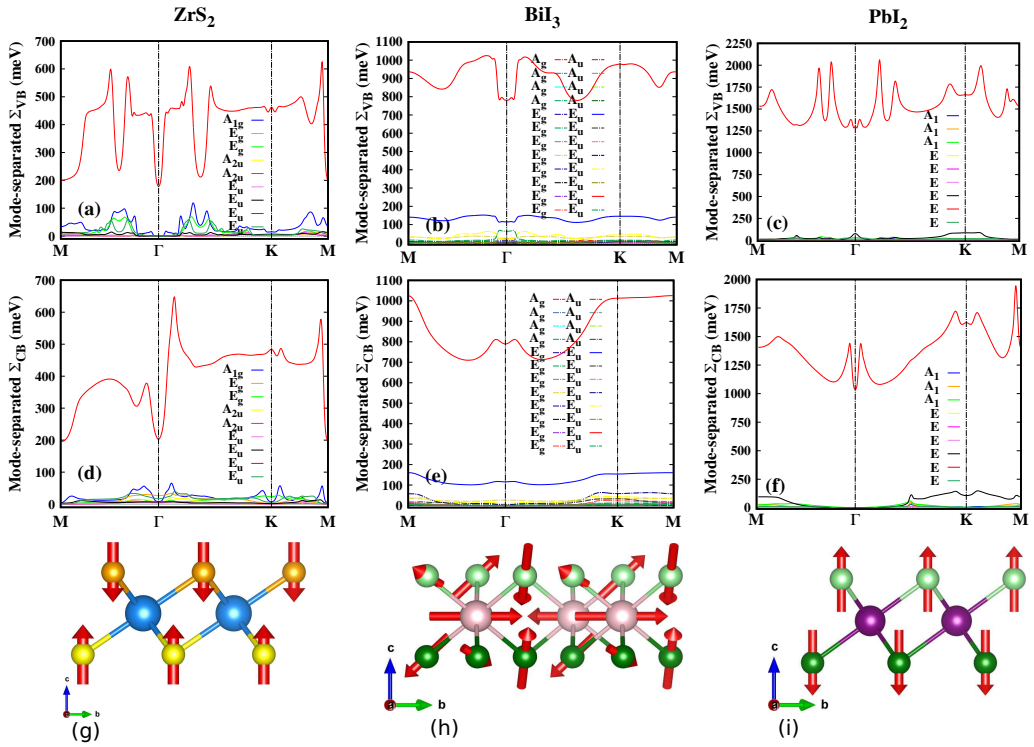

FIG. S1. The mode resolved imaginary part of electron-phonon self energy for the valence (top panels (a-c)) and conduction (middle panels (d-f)) bands for the ML-ZrS_2, ML-BiI_3 and ML-PbI_2 at 300 K, where contribution from various modes are shown by different colors. The largest contribution to $\mathrm{Im}\Sigma_{n,k}$ due to optical modes is shown by red curves in each case. The vibrational patterns of optical modes at Γ point with dominant contribution to $\mathrm{Im}\Sigma_{n,k}$ are shown for ML-ZrS_2, ML-BiI_3 and ML-PbI_2 in (g-i).

[1] Inorganic Chemistry by J. E. Huheey, E. A. Keiter,R. L. Keiter and O. K. Medhi, Pub: Pearson Education India.