Electronic Supplementary Material (ESI) for Inorganic Chemistry Frontiers.

High thermoelectric efficiency in monolayer PbI_2 from 300 K to 900 K

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I. GRÜNEISEN PARAMETERS

The Grüneisen parameter describes the thermal expansion of a crystal on its vibrational properties, and provides information on the anharmonic interactions. A larger Grüneisen parameter indicates stronger anharmonic vibrations. The mode Grüneisen parameters can be calculated as[1]

$$\gamma_p(\mathbf{q}) = -\frac{1}{6\omega_p^2(\mathbf{q})} \sum_{\eta' l'} \sum_{\eta'' l''} \sum_{\alpha\beta\gamma} \Phi_{\alpha\beta\gamma}^{\eta 0, \eta' l', \eta'' l''} \frac{e_{\alpha\eta}^p(\mathbf{q}^*) e_{\beta\eta'}^p(\mathbf{q})}{\sqrt{M_\eta M_{\eta'}}} e^{i\mathbf{q}\cdot\mathbf{R}'_l} \mathbf{r}_{\eta'' l'' \gamma}, \quad (1)$$

where α, β and γ are the Cartesian components, $e_{\alpha\eta}^p(\mathbf{q}^*)$ and $e_{\beta\eta'}^p(\mathbf{q})$ are the phonon eigenvectors, and $\mathbf{r}_{\eta l \gamma}$ is the position of η^{th} atom in l^{th} primitive cell. As shown in Figure S1, the mode Grüneisen parameters of PbI_2 are comparable to those of PbTe[2], indicating strong anharmonicity.

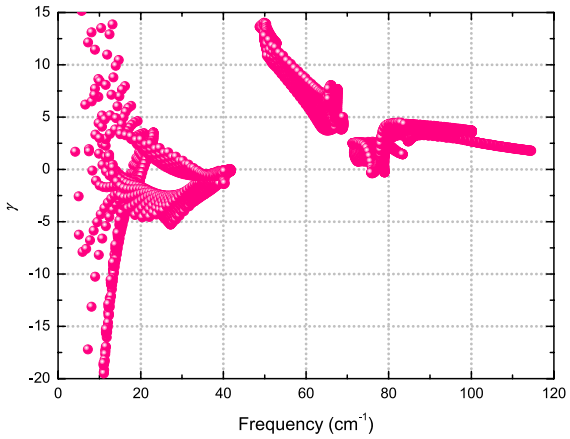

FIG. 1. mode Grüneisen parameter for PbI_2 with respect to phonon frequency.

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