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

\[ \gamma_p(q) = -\frac{1}{6\omega_p^2(q)} \sum_{\eta'\eta''} \sum_{\alpha\beta\gamma} \Phi_{\eta\eta',\eta''}^{\alpha\beta\gamma} \frac{e^p_\alpha(q^*)e^p_\beta(q)}{\sqrt{M_\eta M_{\eta'}}} e^{iq} R_{\eta'} r_{\eta''\gamma}, \]  

where \( \alpha, \beta \) and \( \gamma \) are the Cartesian components, \( e^p_\alpha(q^*) \) and \( e^p_\beta(q) \) are the phonon eigenvectors, and \( r_{\eta l} \) is the position of the \( \eta \)th atom in the \( l \)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.
REFERENCES