Anharmonic thermodynamic properties and phase boundary across the post-perovskite transition in $MgSiO_3$

Zhen Zhang[1] and Renata M. Wentzcovitch[1]

[1]Department of Applied Physics and Applied Mathematics, Columbia University, New York, NY 10027, USA.

Method: phonon quasiparticle approach

Mode-projected velocity autocorrelation function:

$$\langle V_{\mathbf{q}s}(0)\cdot V_{\mathbf{q}s}(t)\rangle = \lim_{\tau\to\infty}\frac{1}{\tau}\int_0^{\tau} V^*_{\mathbf{q}s}(t')V_{\mathbf{q}s}(t'+t)dt'$$

$$V_{\mathbf{q}s}(t) = \sum_{i=1}^{N}\sqrt{M_i}\mathbf{v}_i(\mathrm{t})e^{i\mathbf{q}\cdot\mathbf{R}_i}\cdot\hat{\mathbf{e}}_{\mathbf{q}s}$$

Renormalized frequency and phonon linewidth:

$$\langle V_{\mathbf{q}s}(0)\cdot V_{\mathbf{q}s}(t)\rangle = A_{\mathbf{q}s}\cos(\tilde{\omega}_{\mathbf{q}s}t)e^{-\Gamma_{\mathbf{q}s}t}$$

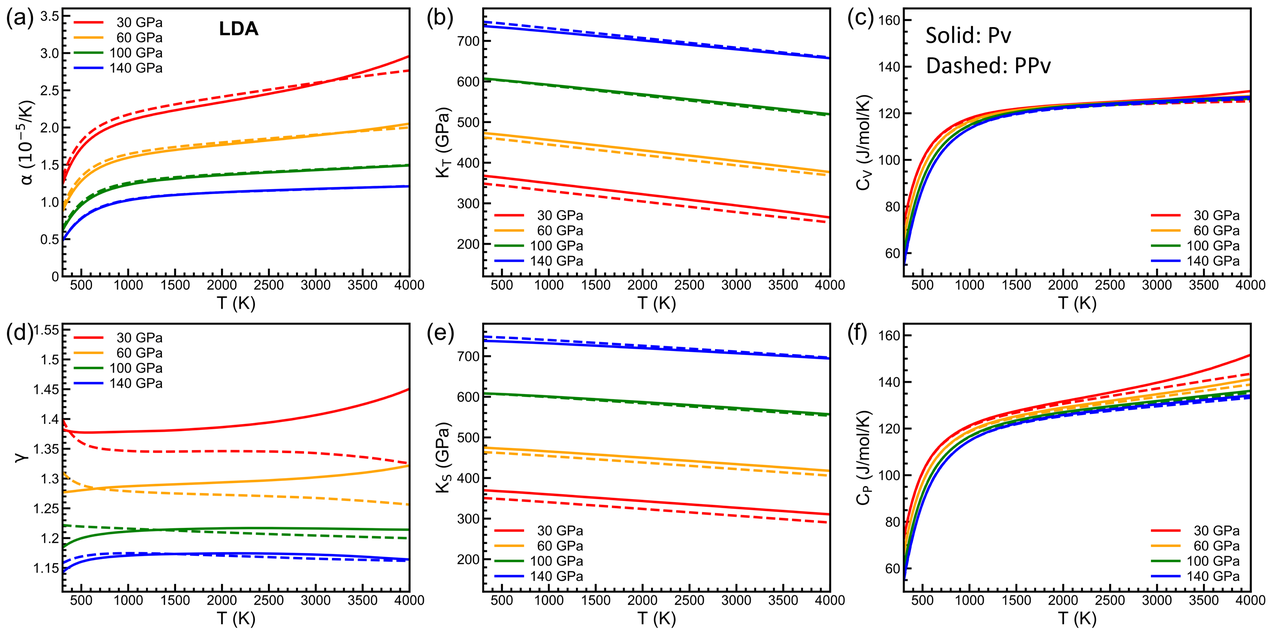
$$G_{\mathbf{q}s}(\omega) = \left|\int_0^{\infty}\langle V_{\mathbf{q}s}(0)\cdot V_{\mathbf{q}s}(t)\rangle e^{i\omega t}dt\right|^2$$

Vibrational entropy and free energy with the PGM:

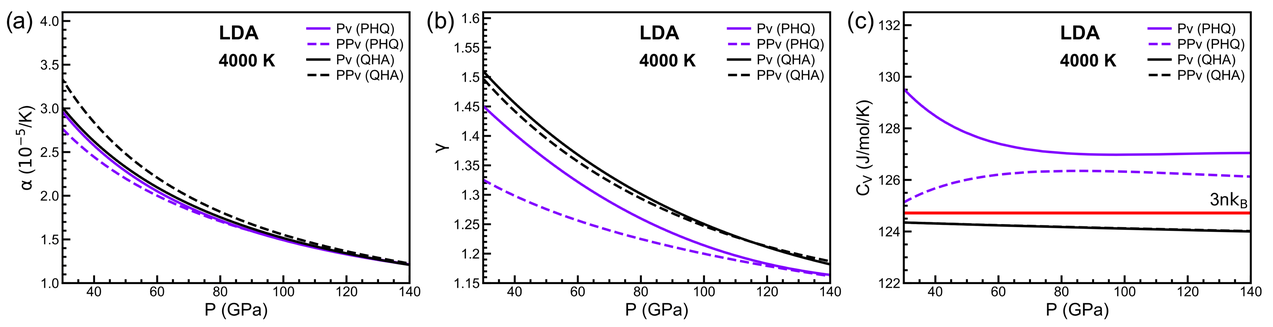
$$S_{\mathrm{vib}}(T) = k_{\mathrm{B}}\sum_{\mathbf{q}s}[(n_{\mathbf{q}s}+1)\ln(n_{\mathbf{q}s}+1) - n_{\mathbf{q}s}\ln n_{\mathbf{q}s}]$$

$$F(T) = E_0 + \tfrac{1}{2}\textstyle\sum_{\mathbf{q}s}\hbar\omega_{\mathbf{q}s} - \int_0^T S_{\mathrm{vib}}(T')dT'$$

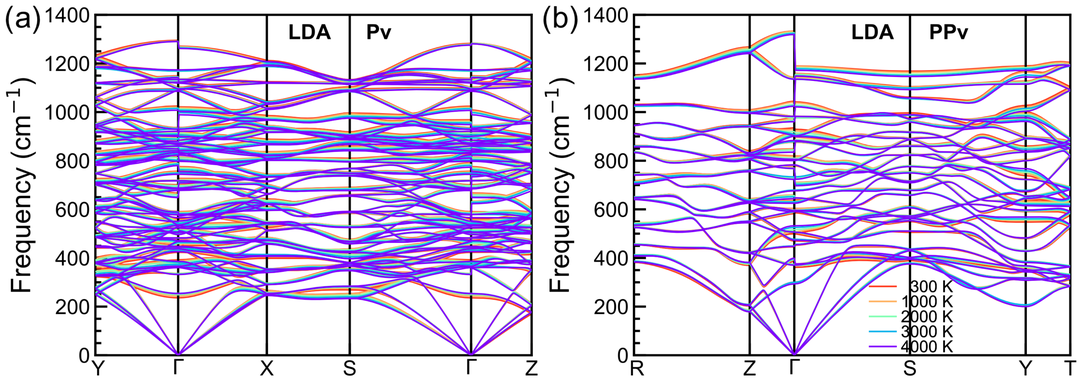
Anharmonic thermodynamic properties



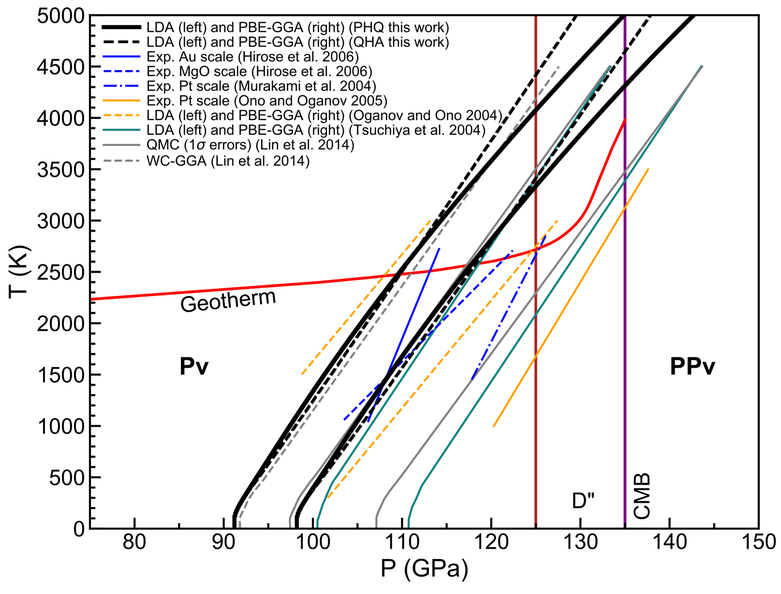
PHQ and QHA comparisons



T-dependent anharmonic phonon dispersions



Pv-PPv phase boundaries



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