

Abstract Submitted  
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**Anharmonic Phonons in Complex Systems: Application to MgSiO<sub>3</sub>-Perovskite** DONG-BO ZHANG, TAO SUN, RENATA WENTZCOVITCH, University of Minnesota — We propose a strategy to capture phonon frequency renormalization due to phonon-phonon interactions included in molecular dynamics simulations (self-consistent phonons). This strategy is effective irrespective of crystal structure complexity and facilitates the Fourier interpolation of anharmonic frequencies throughout the Brillouin zone. Calculation of anharmonic frequency shifts in MgSiO<sub>3</sub>-perovskite validates the method by reproducing well irregular thermal shifts measured by Raman spectroscopy at ambient conditions.  
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