Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Phonon Quasi-Particles and Anharmonic Free Energy in Complex Systems[1] DONG-BO ZHANG, TAO SUN, RENATA WENTZCOVITCH, University of Minnesota, Twin Cities, MN 55455 — We use a hybrid strategy to obtain anharmonic frequency shifts and lifetimes of phonon quasi-particles from first principles molecular dynamics simulations in modest size supercells. This approach is effective irrespective of crystal structure complexity and facilitates calculation of full anharmonic phonon dispersions, as long as phonon quasi-particles are well defined. We validate this approach to obtaining anharmonic effects with calculations in $MgSiO_3$-perovskite, the major Earth forming mineral phase. First, we reproduce irregular temperature induced frequency shifts of well characterized Raman modes. Second, we combine the phonon gas model (PGM) with quasi-particle frequencies and reproduce free energies obtained using a direct approach such as thermodynamic integration. Using thoroughly sampled quasi-particle dispersions with the PGM we then obtain first-principles anharmonic free energy in the thermodynamic limit ($N \rightarrow \infty$).

[1]Research supported by Abu Dhabi-Minnesota Institute for Research Excellence (ADMIRE) and NSF grant EAR-1047629.

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Date submitted: 15 Nov 2013 Electronic form version 1.4