Abstract Submitted
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High-throughout thermodynamics of vibrational degrees of freedom with AFLOW PINKU NATH, JOSE J. PLATA, CORMAC TOHER, STEFANO CURTAROLO, Duke University, MEMS Department — Phonons are responsible for many thermodynamic properties of the materials. Quasiharmonic approximations have been used successfully as a strong theory in order 'to incorporate phonon contributions to material properties [1]. We have implemented this method to calculate Gruneisen parameter (GP) which captures the properties related to thermal variations and connects two important thermodynamic variables such as isobaric and isochoric specifics heat. This method has been implemented in AFLOW framework for high-throughput computational materials science to accelerate the discovery of new materials and properties interesting for industries. GP has been calculated with the derivative of the frequency and the Feynman-Hellman technique, and the results for both techniques are consistent. We have also calculated coefficient of thermal expansion and bulk modulus using a quadratic fit followed by Birch Murnaghan fit of volume-energy data. For a large set of the materials tested, our results are in agreement with the experimental data.

[1] C. Toher, et. al, Phys. Rev. B 90, 174107, 2014.

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