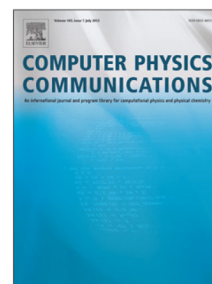


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An open-source implementation of a quasi harmonic approach to compute the
intramolecular entropy of particle systems

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Keywords: Intramolecular Entropy; Quasi Harmonic method; Atomistic and Coarse Grained Resolution; Temperature dependence; Molecular Dynamics

Abstract

The implementation of a quasi harmonic approach to determine the intramolecular entropy of particle systems in an open-source python code is presented. The code makes use of platform-independent tools and can be readily transferred to any computer platform which can run python. It is straightforward to incorporate the code into the LAMMPS software as well as into other molecular simulation programs. In

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