a-TDEP : Temperature Dependent Effective Potential for ABINIT

F. Bottin[1], J. Bouchet[1] and J. Bieder[1,2]

[1] CEA, DAM, DIF, F-91297 Arpajon, France.
[2] Theoretical Materials Physics, Q-MAT, CESAM, Universitè de Liège, Belgium

The capture of thermal effects in solid state physic is a long standing issue and several stand-alone or post-process computational codes now include the so called anharmonic effects. We show how A-TDEP can produce a large panel of temperature dependent thermodynamic quantities, from a single *ab initio* molecular dynamic trajectory and by means of a Graphical User Interface (AGATHE) very easy to use : phonon spectra, free energy, specific heat, elastic constants and moduli, Grüneisen parameter, thermal expansion, sound velocities... We start by detailing how the originally "Temperature Dependent Effective Potential" method proposed by Hellman *al.* [1] is implemented in ABINIT [2]. In particular, we present the various algorithms and schemes used to obtain the Interatomic Force Constants : self-consistency, constrained least-square method, lattice symmetries, translation or rotation invariances of the system... We also show some representative applications of A-TDEP (Ti, U, Fe, MgO, Pu...) [3], and highlight how the strong anharmonicity alters their thermodynamic properties.

References

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