

O.39 aTDEP : Lattice dynamics including anharmonicity

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The evaluation of thermal effects is a long standing issue in solid state physics. If most of usual implicit effects can be taken into account in the framework of quasi-harmonic approximation (QHA), the explicit effects cannot be described without a treatment going beyond the QHA approach. Since the 60's, several microscopic formalisms have been proposed and, during the last ten years, a few computational methods has been developed. In this talk, we discuss our implementation of one of them, the "Temperature Dependent Effective Potential" (TDEP) [1] in the ABINIT package [2].

In particular, we show how ATDEP can produce a large panel of thermodynamic quantities including explicit thermal effects : phonon spectra, free energy, specific heat, elastic moduli, Grüneisen parameter, thermal expansion, sound velocities... In particular, we focus on the 2nd, 3rd and 4th order Interatomic Force Constants, which are the key ingredients behind all these thermodynamic quantities. At last, we present some representative applications of ATDEP [3] and highlight how the strong anharmonicity alters the thermodynamic properties.

[1] O. Hellman, I.A. Abrikosov, S.I. Simak, Phys. Rev. B **84**, 180301(R) (2011); O. Hellman, I.A. Abrikosov, Phys. Rev. B **88**, 144301 (2013).

[2] J. Bouchet and F. Bottin, Phys. Rev. B **92**, 174108 (2015); F. Bottin, J. Bieder and J. Bouchet, Comput. Phys. Commun. **254**, 107301 (2020).

[3] A. Dewaele, V. Stutzmann, J. Bouchet, F. Bottin, F. Occelli, M. Mezouar, Phys. Rev. B **91**, 134108 (2015); J. Bouchet, F. Bottin, Phys. Rev. B **95**, 054113 (2017); B. Dorado, F. Bottin, J. Bouchet, Phys. Rev. B **95**, 104303 (2017); J. Bouchet, F. Bottin, V. Recoules, F. Remus, G. Morard, R.M. Bolis, A. Benuzzi-Mounaix, Phys. Rev. B **99**, 094113 (2019); S. Anzellini, F. Bottin, J. Bouchet and A. Dewaele, Phys. Rev. B **102**, 184105 (2020).