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 effects can be taken into account in the framework of harmonic or quasi-harmonic approximation (QHA), some strong or subtle explicit effects cannot be described without a treatment going beyond the QHA approach. Since the beginning of the 60's, several microscopic formalisms has been proposed and, during the last ten years, a few computational methods has been developed in order to include the calculation of intrinsic thermal effects. One of them, named "Temperature Dependent Effective Potential" (TDEP), has been proposed by O. Hellman *al.* [1] and is able to capture such anharmonic effects. More recently, we have performed an implementation of this method in the *ab initio* package ABINIT [2].
In this talk, we show how A-TDEP can produce a large panel of thermodynamic quantities including explicit thermal effects, starting from a single *ab initio* molecular dynamic trajectory : phonon spectra, free energy, specific heat, elastic constants and moduli, Grüneisen parameter, thermal expansion, sound velocities... In particular, we will focus on the 2^{nd}, 3^{rd}, 4^{th}... order Interatomic Force Constants (IFC), which are the key ingredients behind all these thermodynamic quantities. At last, we present some representative applications of A-TDEP (Ti, U, Si, Zr, Fe, MgO, Pu...) [3], and highlight how the strong anharmonicity alters their thermodynamic properties.

References

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