

Computing thermo-elasticity of crystalline systems from quasi-static and quasi-harmonic approximations

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An effective algorithm for the quasi-harmonic calculation of anisotropic thermo-elasticity of materials is discussed and implemented into the CRYSTAL program for quantum-mechanical simulations of extended systems. The directional elastic response of solid compounds is expressed in terms of the fourth-order *stiffness tensor*: its components – namely, the elastic constants – define the stress-strain linear relationships.

One of the main challenges to state-of-the-art methodologies is that of reliably and efficiently accounting for thermal effects on solid compounds. The simplest way to accomplish this is by means of standard harmonic lattice dynamics; however, when anharmonic thermal effects are totally neglected, the volume and elastic response do not exhibit any dependence on the temperature. An easy way to overcome these limitations is offered by the so-called *quasi-harmonic approximation*: it explicitly introduces the volume into the expression of the phonon frequencies, which are still computed at the harmonic level but at several volumes. The Helmholtz free energy is then expressed as function of both volume and temperature (and not just of temperature as it would be at the harmonic level), thus allowing the thermal expansion of the system to be determined. Then, the thermo-elastic constants of the compound are given by the second-order derivatives of the

Helmholtz free energy with respect to strain – normalized by the volume at that temperature. A simpler approach is also presented: inside the *quasi-static approximation*, the thermal dependence of elastic constants is assumed to be due only to the thermal expansion of the system – the derivatives are performed on the static energy, which does not include any thermal contribution. This algorithm has then been applied to the forsterite mineral and the results are discussed: it shows great accuracy with experimental data (especially with the trends) and good coherency among different DFT functionals.

Speaker Biography

Maurizio Destefanis obtained his BSc and MSc in Chemistry at University of Turin, Italy. During the degree program, his interests were focused on the interface between chemistry and computer science, since he developed software for chemistry during both his theses projects and research activity in computational chemistry. He specialized into algorithm development (mainly through the Fortran programming language – imperative and static) and application design (mainly through the Ruby programming language – object-oriented and dynamic). Currently, he is working in the Information Technology field for the company Accenture as a backend Java developer. In 2011, he was also awarded by the Italian Chemical Society with the bronze medal at the Italian Chemistry Olympiads competition.

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