

"ANHARMONISITY AND EXAFS STUDIES BEYOND THE QUASIHARMONIC APPROXIMATION"



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Anharmonicity of lattice dynamics is very important in relation to many effects in crystals as thermal expansion, structural phase transitions, soft modes in ferroelectrics and related HTSC phenomena. In strongly anharmonic systems the so-called explicit anharmonicity effect links the phonon frequencies and interatomic forces to the amplitude of the atomic vibrations that is realised in the ab-initio calculations beyond quasiharmonic approximation (BQHA).

Femtometer accuracy in the determination of interatomic distances by EXAFS measurements is now attainable [1-4], therefore additional information on the lattice dynamics can be obtained from EXAFS spectra. We propose an approach [3] beyond the quasiharmonic approximation for the interpretation of original EXAFS, neutron PDOS, Raman and infrared data. Ab initio BQHA calculations of electronic and vibration properties are performed not at the equilibrium positions atoms but at the most probable positions for a given temperature, one can obtain from EXAFS data that describes the system at elevated temperatures.

References

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