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Ab Initio Computation of Phonon-Phonon and Magnon-Phonon Interactions: Successes and Challenges

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A key requirement in developing systematic approaches to explore and predict properties of materials not yet synthesized is the availability of accurate computational tools determining energies not only at T = 0 K but also under realistic finite temperature conditions. A critical step towards this goal is the ability to accurately describe all relevant excitation mechanisms such as phonons, magnons, excited electrons. For many scientifically and technologically important functional as well as structural materials the various excitation mechanisms are not adiabatically decoupled but non-adiabatic couplings e.g. between magnons and phonons or between electrons and photons (electron-phonon interaction) become critical and need to be included for an accurate description of their thermodynamic properties.
In the talk we will show how novel sampling strategies in the atomic configuration space together with techniques to address the spin-degrees of freedom including spin-quantization in magnetic materials allow an unbiased and accurate determination of all relevant temperature dependent free energy contributions. While in the past the focus has been mainly on the quasiharmonic contributions (which are computationally most easily to obtain) recent advances provide now for the first time the opportunity to systematically include anharmonic and magnetic contributions all the way up to the melting temperature. The flexibility and the predictive power of these approaches to describe these complex excitation and coupling mechanisms will be discussed for selected materials such as ultra-high strength steels, magnetic shape memory alloys or lightweight alloys.

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