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Title: Fully ab initio determination of free energies: Methodological challenges and applications

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The combination of accurate first principles calculations with mesoscopic/macroscopic thermodynamic and/or kinetic concepts has quickly advanced in the past few years and allows now to tackle even the complexity of advanced engineering materials. Key to these studies is the highly accurate determination of free energies. In the talk we will show how efficient sampling strategies together with high convergence density-functional theory calculations 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) new advances in methods and computational power provide now for the first time the opportunity to systematically include anharmonic and magnetic contributions. The flexibility and the predictive power of this approach will be discussed for examples relevant to the design and understanding of modern high strength steels or light weight metallic alloys.