

Abstract Submitted  
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**Ab initio determination of the magnetic free energy contribution of metallic systems** FRITZ KÖRMANN, ALEXEY DICK, BLAZEJ GRABOWSKI, TILMANN HICKEL, JÖRG NEUGEBAUER, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany — An accurate prediction of the free energy is the basis to compute phase diagrams, finite temperature materials parameters, or kinetic barriers and is thus fundamental in computational materials design. One of the most challenging contributions - but crucial for many engineering materials - is the magnetic entropy. The most popular ab initio approach for the latter is the use of an effective Heisenberg model solved using classical Monte Carlo (cMC) approaches and neglecting quantum effects. We discuss the impact of the latter based on extensive model calculations where Quantum MC calculations are available. An empirical rescaling scheme is derived allowing to considerably improve the cMC. The method is applicable to strong ferromagnetic systems with magnetic frustration is absent or weak. The application and performance of the new approach is demonstrated for pure Fe.

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