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Title: Simple Heisenberg model based method to accelerate first-principle thermodynamics simulations for magnetic systems.

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Thermodynamic properties of magnetic materials based on first-principle statistical mechanics (Wang-Landau/Local Self Consistent Multiple Scattering methods) are well designed to take advantage of the recent developments in the computational science and technology but require very large computational resources. We deploy a simple fitting procedure based on an Heisenberg type Hamiltonian in order to accelerate the convergence of the magnetic spin space sampling. On a representative set of magnetic configurations, the method minimizes the difference between the first-principles energies and the model Heisenberg energies based on the model exchange interactions. The subset is significantly smaller than the set required by a direct sampling with the Wang-Landau procedure. The crux of the method is that the uniformly distributed configurations from the classical Hamiltonian can then be used to restart the calculation for the first-principles Hamiltonian in a more advanced state of convergence.