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Spin disorder effect on the electronic and transport properties in magnetic materials from first principles

The formation of a spin-disordered state due to the local moment fluctuations at elevated temperatures strongly affects the ground state electronic properties of magnetic materials. In particular, we investigate how the spectral function changes as a function of temperature in selected Heusler alloys. Furthermore, we focus on the spin disorder effect on the thermoelectric and spin-caloric transport properties in various magnetic nanostructures. This is motivated by the miniaturization of spintronics devices and by recent suggestions that magnetic nanostructures can lead to extraordinary thermoelectric effects due to quantum confinement [1].

In our approach, the electronic structure is calculated within the full-potential Korringa-Kohn-Rostoker Green function (KKR-GF) framework [2] using the local density approximation. The Monte-Carlo methodology is used to simulate the effect of temperature induced spin disorder and the set of spin-disordered configurations is fed back in the KKR-GF method to obtain the statistical average of the relevant material properties [3-5].


All interested are cordially welcome!