Spin transport and spin-caloric effects in (Cr,Zn)Te half-metallic nanostructures: Effect of spin disorder at elevated temperatures from first principles

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An important contribution to the thermoelectric and spin-caloric transport properties in magnetic materials at elevated temperatures is the spin-disordered state formation due to the local moment fluctuations. This effect has not been largely investigated so far. Motivated by the miniaturization of spintronics devices and a possible enhancement of thermoelectric effects due to quantum confinement, we focus on CrTe half-metallic ferromagnetic nanostructures (thin layers, nanowires) embedded in ZnTe matrix and contacted by Ag leads. The electronic structure is calculated within the full-potential Korringa-Kohn-Rostoker Green function framework. The temperature induced spin disorder is simulated by the Monte-Carlo methodology and the Landauer-Büttiker approach is used to evaluate the transport properties. The thermoelectric and spin-caloric coefficients can be reduced, enhanced or even change sign due to the spin-disorder depending on temperature and the particular nanostructure geometry. Our calculations show these effects for the first time [1,2]. Furthermore, we show that substitutional impurities in CrTe nanowires could considerably enhance the thermoelectric figure of merit [2]. Support from DFG (SPP1538) is gratefully acknowledged.

[1] Kováčik R. et al., Phys. Rev. B 89, 134417, (2014)
[2] Kováčik R. et al., Phys. Rev. B 91, 014421, (2015)