Seminar: Hard Condensed Matter Theory

JOHANNES GUTENBERG UNIVERSITÄT MAINZ

Room: Galilei Raum, 01-128 (Staudinger Weg 9)
Time: October 17th, 2017 at 14:00

Roman Kováčik

Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52428, Jülich, Germany

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].

[1] N. Vu et al., APEX 4, 015203 (2011).
[2] N. Papanikolaou et al., J. Phys.: Condens. Matter 14, 2799, (2002), also see: kkr-gf.org.
[3] Ph. Mavropoulos et al., Phys. Rev. B 69, 125104, (2004).
[4] R. Kováčik et al., Phys. Rev. B 89, 134417, (2014).
[5] R. Kováčik et al., Phys. Rev. B 91, 014421, (2015).

All interested are cordially welcome!
