

Colloquium on Solid-State Physics

Date: Thursday, Nov 17, 2011

Time: 17.15 h
Coffee, tea and cookies at 17.00h in front of the lecture hall

Place: Hörsaal HS 3
Physik - Department
Technische Universität München



Seminar of the Collaborative Research Centre/Transregio TRR 80:

Origin of the ferromagnetic spin coupling and the role of electronic correlations in N-doped MgO

Dr. Marjana Ležaić, PGI-1, Forschungszentrum Jülich, D-52425 Jülich, Germany

In the past few years there is a growing interest in engineering a ferromagnetic state in otherwise nonmagnetic insulators by doping with sp elements instead of transition-metal doping that is traditionally used in diluted magnetic semiconductors. This novel magnetic materials design was stimulated by several unexpected experimental observations of room-temperature ferromagnetism in highly defective wide-gap semiconductors and insulators and is particularly interesting, both from fundamental and practical points of view. We discuss possible d^0 -magnetism in N-doped MgO, using first principles calculations and consider two limits: the one of weak on-site electron correlations (within the GGA approach) and the one of strong correlations (within the GGA+U approach). The two limits yield two different exchange mechanisms that possibly stabilize the ferromagnetic state. In the case of weak correlations a spin-polarized impurity band emerges close to the MgO valence band, with a ferromagnetic state stabilized by the double-exchange mechanism [1]. When strong correlations are taken into account, a special orbital arrangement of the unoccupied $2p$ -orbitals on N-impurities is achieved due to a weak intersite Coulomb interaction; in such a state, the kinetic exchange favors a ferromagnetic spin coupling [2]. The strength of the exchange interactions in the two limits and the possibility of achieving a high magnetic ordering temperature will be discussed.

1. Ph. Mavropoulos, M. Ležaić, and S. Blügel, Phys. Rev. B 80, 184403 (2009).
2. I. Slipukhina, Ph. Mavropoulos, S. Blügel, and M. Ležaić, Phys. Rev. Lett. 107, 137203 (2011).