SFB 608

Einladung zum Kolloquium

Ort: Universität zu Köln
II. Physikalisches Institut, Seminarraum 201

Zeit: Mittwoch**,** 23.07.03, 15 Uhr c.t.

Sprecher: Professor S.G. Ovchinnikov
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Thema: **The electronic energy structure of $FeBO_3$ and its change under high pressure in the multi-electron approach taking into account strong electron correlations**

Abstract of the talk:

A multi-electron model of the electronic structure for $FeBO_3$ is presented. The bottom of the conductivity band and the top of the valence band are formed by s,p electrons of the BO_3 group, and in the wide energy gap there are d-levels of 3d-ion. These levels are calculated as d-resonances between the multi-electron terms of d(n) configurations. Local d-resonances $E(d^6)$-$E(d^5)$ and $E(d^5)$-$E(d^4)$ are calculated resulting in adding and removing one d-electron to Fe^{+3} ion, and the scheme of the density of states is constructed in good agreement to optical absorption spectra. According to this scheme $FeBO_3$ is a charge-transfer insulator. Under external pressure the crystal field parameter 10Dq increases, and at some critical value the crossover of high-spin 5/2 to low-spin 1/2 takes place. In the high-pressure phase the change of the energy level scheme results in a smaller value of the semiconducting energy gap. The magnetic properties of the high-pressure phase are predicted to be antiferromagnet with S=1/2 and a low Neel temperature.