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.