THE ELECTRONIC STRUCTURE OF THE RMn_2Ge_2 (R = Ca, Y, Ba, La) ANTIFERROMAGNETS

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9.7 cm

We present the electronic structure of the tetragonal RMn_2Ge_2 (R=Ca,Y,Ba,La) antiferromagnets investigated by the selfconsistent KKR calculations. In the above-mentioned compounds the two types of antiferromagnetic structure (AF_1 and AF_2) were experimentally detected. In YMn_2Ge_2 the Mn magnetic moments are arranged parallel in the a-b plane, while antiferromagnetically inter the a-b planes (AF_1). On the contrary, in $CaMn_2Ge_2$, $LaMn_2Ge_2$ and $BaMn_2Ge_2$, the neighboring μ_{Mn} (in the a-b plane) are aligned anti-parallel (AF_2). Moreover, the ordering of the Mn magnetic moment in RMn_2Ge_2 seems to be governed by the Mn-Mn distance d_{in} in the a-b plane. For $d_{in} < 2.87$ Åthe AF_1-type of magnetic arrangement is observed, otherwise ($d_{in} \geq 2.87$Å) the AF_2-type occurs. The KKR results of the RMn_2Ge_2 compounds show that the μ_{Mn} value increases more or less linearly with d_{in}. The calculated magnetic moments on Mn: $2.17\mu_B$ (YMn_2Ge_2), $2.74\mu_B$ ($CaMn_2Ge_2$), $2.95\mu_B$ ($LaMn_2Ge_2$) and $3.47\mu_B$ ($BaMn_2Ge_2$) remain in good agreement with the neutron diffraction measurements (in μ_B): 2.20, 2.67, 3.05, 3.66, respectively. The reason for the changing of the AF-type structure, near $d_{in} = 2.87$Å, is discussed in a view of the total energy KKR computations.

13.4 cm

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