The spin state issue in the $R$BaCo$_2$O$_{5.5}$ cobaltates

HUA WU, Z. HU, T. BURNUS, D. I. KHOMSKII, L. H. TJENG, Institute of Physics II, University of Cologne, Germany — The double perovskites $R$BaCo$_2$O$_{5+\delta}$ ($R$=rare earth, $0 \leq \delta \leq 1$) display intriguing phenomena such as charge and orbital ordering, as well as antiferromagnetic to ferromagnetic transition, depending on the oxygen concentration. In particular, the $\delta=0.5$ system shows a giant magnetoresistance effect, and its metal-insulator transition has been often interpreted in terms of a spin-state transition [1,2], which, however, is fiercely debated [3,4]. To address the spin-state issue, we performed density-functional theory calculations which include a mean-field correction for the correlation effects caused by the Co 3$d$ electrons. We have investigated various scenarios with different combinations of the low-, intermediate- and high-spin (LS, IS, and HS) states. Our results show that the pyramidally coordinated Co$^{3+}$ ions are exclusively in the HS state since [3], in disagreement with [1,2]. The octahedrally coordinated Co$^{3+}$ can be stabilized into a LS-HS ordered state if we take into account the superstructure recently reported [4]. Our results put limits as to how much spin-state transition could accompany the metal-insulator transition. [1] C. Frontera et al., Phys. Rev. B 65, 180405(R) (2002). [2] A. A. Taskin et al., Phys. Rev. Lett. 90, 227201 (2003). [3] Z. Hu et al., Phys. Rev. Lett. 92, 207402 (2004). [4] D. D. Khalyavin et al., Phys. Rev. B 75, 134407 (2007)