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The spin state issue in the RBaCo$_2$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 RBaCo$_2$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 δ=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 3d 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)

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