MAGNETISM AND ELECTRONIC STRUCTURE OF $LaCoO_3$

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$LaCoO_3$ exhibits unusual magnetic properties intriguing the magnetic society by more than 30 years, after pioneering works of Goodenough (*Phys.Rev.* **155** (1967) 932). $LaCoO_3$ show a diamagnetic low-temperature state that seems to transform with temperature into a magnetic state. It is often discussed in terms of low-spin and high-spin states. Recently an intemediate-spin state has been additionally postulated to exist (*Phys.Rev.* B **54** (1996) 5309).
We have performed calculations of the fine electronic structure of the Co^{3+} ion in the perovskite-like structure of $LaCoO_3$. We have found that the diamagnetic state of $LaCoO_3$ is related with the non-magnetic state of the Co^{3+} ion in the atomic scale. Moreover, we have found microscopic picture for the existence of the low-, intermediate- and high-spin states of the cobalt ions and their transformation with temperature. Very strong correlation between the local magnetism, the local crystallographic symmetry (Jahn-Teller effect) and the fine electronic structure has been found.
The present results confirm the importance of the spin-orbit interactions on the 3d-ion moment and can enlighten mechanisms responsible for the formation of 3d magnetic moments.

9.7 cm

13.4 cm

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