Seminář oddělení magnetik a supravodičů
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Dynamical mean field modeling of $LaCoO_3$

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Abstract. The interest in $LaCoO_3$ arises from its complex magnetic and transport properties. The low-temperature $LaCoO_3$ is a non-magnetic insulator. Above 100 K it transforms into a paramagnetic insulator and the metal-insulator crossover takes place around 500 K. The ionic state of Co in this compound is Co^{3+}. The $3d$ orbitals, split to lower three t_{2g} and upper two e_g, accommodate six electrons. Depending on the number of e_g electrons we distinguish the low-spin (LS) state with a spin number $S = 0$, the intermediate spin state (IS, $S = 1$), and the high spin state (HS, $S = 2$). Presently, there are no doubts about prevailing LS character of the low-temperature non-magnetic insulator and the HS character of the paramagnetic metal. Two probable scenarios for the paramagnetic insulator are the LS+HS statistical mixture or the IS. The possibility of the short-range orbitally ordered state with alternating LS+HS and LS sites has also been proposed.
We studied the properties of $LaCoO_3$ with a dynamical mean field theory (DMFT) combined with local density approximation for non-correlated part. We successfully reproduced the metal-insulator transition. The magnetic crossover cannot be modeled as the temperature is too low for employed DMFT expansion, but we were able to stabilize both non-magnetic and paramagnetic state adjusting the exchange interaction parameter J. Our results testify to LS+HS scenario of paramagnetic insulator, but we also observed strong hybridization with oxygen p-orbitals, which increases the mean number of electrons on Co atoms to around 6.7 in the non-magnetic and around 6.4 in the paramagnetic state.