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Journal of Physics: Conference Series 2012 vol.394 N1

Ab-initio investigation of spin states of sodium cobaltate Na 2/3CoO2

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Abstract

Resent experiments in the lamellar system NaxCoO2 detected a transition of Co planes into a puzzling metallic state at x ≥ 2/3, which co-exists with a robust arrangement of the 3d cobalt electrons: The triangular Co lattices are disproportionated in the spinless Co3+ sites (Co1), and Co3.44+ sites (Co2) with enhanced magnetism forming conducting sublattices. This textures concur with a tightening of the ferromagnetic (FM) interaction in planes, and emerge when the sodium ions become arranged in layers in between the CoO2 slabs. In the present research we have investigated ab-initio the appearance of such state in Na2/3CoO2. Towards this end in view we studied an interplay between the electronic coupling to the superstructure of the Na+ ions and local correlations of the itinerant d electrons treated within the GGA+U approximation. Employing the exact crystallographic supercell, the electronic organization has been analyzed upon increasing the energy U of the Coulomb repulsion within the 3d shells at T = 0. The metallic ground state, being a spin density wave with the inplane FM and antiferromagnetic interplane correlations, has been obtained and established to posses two regimes. When U > 2 eV, a crossover develops from a uniform state of the d-lattice to the regular phase with the spin/charge disproportionation between the sites. In particular at the representative value U = 5 eV, the Co13+ sites with suppressed magnetism appears, while the spin-active Co4+ holes are accumulated by the Co2 sites. A related formation of an isolated, narrow conduction band at the Fermi level implies a considerable enhancement of the electron correlations in the crystal field imposed by the Na+ patterns.

http://dx.doi.org/10.1088/1742-6596/394/1/012019