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Disproportionation, Metal-Insulator Transition, and Critical Interaction Strength in $Na_{1/2}CoO_2$[1]

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Spontaneous breaking of symmetry is one of the key concepts of solid state physics related to phase transitions. Charge/spin density wave, or charge/spin ordering if the propagation vector is commensurate, are notorious examples of broken symmetry. The charge disproportionation in $Na_{0.5}CoO_2$ is the main theme of the present work. The results of LDA+U calculations will be presented, exhibiting a charge disproportionation transition at U≈3eV. Na_xCoO_2 attracted considerable attention mainly due to superconductivity of its hydrated form $Na_{0.3}CoO_2.1.3H_2O$ [1]. Besides the superconductivity Na_xCoO_2 exhibits several intriguing properties throughout its phase diagram, such crossover from Pauli-like to Curie-Weiss susceptibility at x=0.5, spin-density wave around x=0.7 or several phase transitions for x=0.5 including metal-insulator transition, charge ordering and magnetic ordering [2]. The Na_xCoO_2 lattice consists of triangular CoO_2 layers separated by Na layer. The mobility of Na ions and fractional occupation of Na sublattice provides an additional complication. Using LDA+U functional within FPLO [3] bandstructure method we have performed series of supercell calculations allowing for breaking of the symmetry between different Co sites. We have found that for large enough, but physically realistic, values of the on-site Coulomb interaction U the Co sublattice disproportionates into sites with formal valencies Co^{4+} and Co^{3+}. We have found that at the same time a gap opens in the excitation spectrum. Details of the bandstructure across the transition as well as the driving forces of the transition in the LDA+U mean field picture will be discussed.

[1] K. Takada *et al.*, Nature (London) **422**, 53 (2003).
[2] M. L. Foo *et al.*, Phys. Rev. Lett. **92**, 247001 (2004).
[3] K. Koepernik and H. Eschrig, Phys. Rev. B **59**, 1743 (1999).

[1]In collaboration with Kwan-Woo Lee and Warren E. Pickett