Charge and Spin Ordering in Insulator Na$_{0.5}$CoO$_2$: Effects of Correlation and Symmetry

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The discovery by Takada and coworkers of superconductivity in Na$_{0.3}$CoO$_2$•$1.3$ H$_2$O near 5K has led to extensive studies of the rich variation of properties in the Na$_x$CoO$_2$ system (0.2 ≤ $x$ ≤ 1), which has a triangular lattice of Co sites and a layered structure. In addition, specifically at $x=0.5$, the system has been observed to undergo a charge disproportionation (2Co$^{3.5+}$ → Co$^{3+}$+Co$^{4+}$) and metal-insulator transition at 50 K, while the rest of the phase diagram is metallic. We will present results of studies of charge disproportionation and charge- and spin-ordering in insulating in Na$_{0.5}$CoO$_2$, applying ab initio band theory including correlations due to intra-atomic repulsion. Various ordering patterns (zigzag and two striped) for four-Co supercells are analyzed before focusing on the observed “out-of-phase stripe” pattern of antiferromagnetic Co$^{4+}$ spins along charge-ordered stripes. This pattern relieves frustration and shows distinct analogies with the cuprate layers: a bipartite lattice of antialigned spins, with axes at 90° angles. Substantial distinctions with cuprates are also discussed, including the tiny gap of a new variant of “charge transfer” type within the Co 3$d$ system.