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Novel electronic states in Na_xCoO_2: Role of strong correlation and Na dopant order

ZIQIANG WANG, Department of Physics, Boston College, Chestnut Hill, MA 02467

We argue that the strong Co intra-atomic Coulomb repulsion renormalizes the crystal field splitting and the bandwidths of the t_{2g} complex in Na_xCoO_2, resulting in a single band crossing the Fermi level at all doping levels x explored by ARPES experiments [1]. On this basis, we study the electronic states using a minimal electron-doped, one-band Hubbard model with large U on the triangular lattice. The important role played by the off-plane Na dopants is taken into account by including the ionic electrostatic potential. We find a class of charge and spin density ordered states where the system alleviates antiferromagnetic (AF) frustration via charge inhomogeneity [2]. We show that the $\sqrt{3} \times 2$ Na order at $x = 0.5$ causes weak $\sqrt{3} \times 1$ charge order in the Co layer and the emergence of AF order with small electron and hole Fermi surface pockets [2]. This theory of the "0.5 phase" is consistent with neutron scattering, NMR, Shubnikov-de Haas oscillations, and transport experiments. In the sodium rich phases, the high density of off-plane Na dopants (or dilute Na vacancies), in their ordered or disordered form, increases the tendency toward carrier localization in the Co plane [3], which competes with in-plane ferromagnetic (FM) correlations described by a renormalized Stoner theory [4]. We argue that the newly discovered electronic phases associated with Na vacancy order [5,6] can be described by a useful notion of "super-Mottness", where strong correlation effects on the superlattice structure give rise to the competition and possible coexistence of localized magnetic moments and itinerant FM carriers.

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