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Charge Disproportionation and Spin Ordering in Na_xCoO_2[1]

WARREN PICKETT, University of California Davis

Observation of strong correlation effects in Na_xCoO_2 for x >0.70 several years ago was followed by observation of superconductivity up to 5 K for x ≈0.3 when the material was hydrated, and then by charge disproportionation, spin ordering, and insulating behavior at x =0.5. The similarities with HTS cuprates are less compelling than the differences, and the first question for theorists is how to understand and describe the electronic system and how it varies with doping. Here we will focus on a description of correlation effects within the correlated band (LDA+U) approach, and compare closely with observed behavior to begin to quantify the strength and character of correlation effects. The x=0 and x=0.5 systems will be given particular atention. At x=0.5, disproportionation and gap opening is followed in detail through a first order charge disproportionation transition $2Co^{3.5+} \rightarrow Co^{3+}+Co^{4+}$ as the correlation strength (U/W) is increased. Comparing with data in the $x \approx 0.3$ regime suggests the system has moved into the multiband regime where the effective Coulomb repulsion becomes $U_{eff} = U/\sqrt{3}$ and strongly lessens correlation effects.

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