

Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Systematic band-filling dependence in the strongly-correlated triangular lattice¹ H. LI, S. MAZUMDAR, U. Arizona, R. T. CLAY, Mississippi State U. — Strongly correlated triangular lattices are of interest because of their applicability to real systems such as superconducting organic charge-transfer solids (CTS) and the hydrated sodium cobaltate. Experimental work on nonhydrated Na_xCoO_2 have found (a) a charge-ordered semiconductor at $x = 0.5$, (b) Curie-Weiss metal for $x > 0.5$, and (c) paramagnetic metal for $x < 0.5$. The strong x -dependence is reminiscent of the band-filling dependence in CTS conductors² We have performed numerical calculations based on the extended Hubbard Hamiltonian to understand the x -dependence. We show that for *finite* Hubbard U , and moderate nearest neighbor interaction V , the normalized probability of double occupancy, which is a measure of the strength of the electron correlation, varies strongly as a function of the density of carriers. We are able to explain (i) the different behavior of $x < 0.5$ and $x > 0.5$, (ii) the absence of the $\sqrt{3} \times \sqrt{3}$ charge-ordering at $x = 1/3$, and (iii) why $x = 0.5$ is unique. Cobalt valence of 3.5 in the superconducting hydrated cobaltate is in agreement with our proposed mechanism of superconductivity in the CTS.³

¹Supported by DOE grant DE-FG02-06ER46315

²S. Mazumdar and A. N. Bloch, Phys. Rev. Lett. **50**, 207 (1983).

³S. Mazumdar and R. T. Clay, Phys. Rev. B **77**, 180515 (R), (2008).

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Date submitted: 20 Nov 2009

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