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The Paired-Electron Crystal in the Two-Dimensional Frustrated Quarter-Filled Band¹ R. T. CLAY, S. DAYAL, Mississippi State University, H. LI, S. MAZUMDAR, University of Arizona — The competition between antiferromagnetic (AFM) and spin-singlet ground states within quantum spin models and the $\frac{1}{2}$ -filled band Hubbard model has received intense scrutiny. Using exact diagonalization and path integral renormalization group (PIRG) calculations we demonstrate a frustration-induced transition from Neel AFM to spin-singlet in the interacting $\frac{1}{4}$ -filled band on an anisotropic triangular lattice. While the AFM state has equal charge densities 0.5 on all sites, the spin-singlet state is a paired-electron crystal (PEC), with pairs of charge-rich sites separated by pairs of charge-poor sites. The PEC provides a natural description of the spin-gapped state proximate to superconductivity (SC) in many organic charge-transfer solids. Our theory explains the semiconducting behavior of $Na_x CoO_2$ at x=0.5, and also applies to spinels isoelectronic with superconducting LiTi₂O₄ and CuRh₂S₄. We discuss recent experimental results in the light of our theory. Pressure-induced SC in these correlated-electron systems is likely a transition from the $\frac{1}{4}$ -filled band valence bond solid to a valence bond liquid.

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