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Magnetic Order-Disorder Transitions on a 1/3 – Depleted Square Lattice H.-M. GUO, T. MENDES, W. E. PICKETT, R. T. SCALETTAR, Department of Physics, UC Davis — Quantum Monte Carlo simulations are used to study the magnetic and transport properties of the Hubbard Model, and its strong coupling Heisenberg limit, on a one-third depleted square lattice. This is the geometry occupied, after charge ordering, by the spin-$\frac{1}{2}$ Ni$ˆ{1+}$ atoms in a single layer of the nickelate materials La$_3$Ni$_2$O$_6$ and La$_4$Ni$_3$O$_8$. Our model is also a description of strained graphene, where a honeycomb lattice has bond strengths which are inequivalent. For the Heisenberg case, we determine the location of the quantum critical point (QCP) where there is an onset of long range antiferromagnetic order (LRAFO), and the magnitude of the order parameter and compare with results of spin wave theory. An ordered phase also exists when electrons are itinerant. In this case, the growth in the antiferromagnetic structure factor roughly coincides with the transition from band insulator to metal in the absence of interactions.

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