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Finite-temperature Quantum Monte Carlo study of a molecular spin ladder[1] SAURABH DAYAL, R.T. CLAY, Department of Physics and Astronomy and HPCC Center for Computational Sciences, Mississippi State University, MS, 39762 — Materials with *ladder* crystal structures consist of two or more coupled one dimensional (1D) chains of atoms or molecules. An example is $(DTTTF)_2M(mnt)_2$, which is a two-leg molecular ladder material that is very similar to many of the molecular *organic* superconductors. These ladder systems have several interesting properties that occur as the temperature(T) is lowered including a spin gap and structural distortions. Furthermore, small physical or chemical changes can lead to a large change in the T-dependence of their electronic properties. Two different theoretical models have been presented to understand these materials, the rectangular and zigzag lattices. To understand the magnetic and charge response functions of these two possible models, we have performed T-dependent Quantum Monte Carlo calculations that incorporate electron-electron interactions need to correctly generate the spin gap. Charge, spin and bond order susceptibilities of an extended Hubbard model with on-site Coulomb repulsion U at quarter filling were calculated for several different model lattice sizes. We investigate the charge ordering and bond distortion patterns within this model.

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