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Temperature dependent competition between charge-ordering and spin-Peierls transition in $(TMTTF)_2X$: the role of quantum phonons[1]

R. T. CLAY, Mississippi State University, R. P. HARDIKAR, Mississippi State University, S. MAZUMDAR, University of Arizona — The $(TMTTF)_2X$ salts are quasi-one-dimensional materials with complex phase diagrams that feature a large number of ordered states including superconductivity. The ground states of these materials are often spin-Peierls (SP) states. However, at intermediate temperatures (100 K) a transition to a charge ordered state is also present, which may compete with the ground state SP ordering. We investigate numerically models for these materials that include three components: electronic interactions, bond-coupled phonons, and Holstein-type phonons coupled to the local charge density. These three components have different energy scales are hence expected to dominate at different temperatures. We explicitely include finite phonon frequency in our calculations using quantum Monte Carlo methods. We present charge, spin, and bond susceptibilities as a function of temperature and discuss recent experiments on these materials.

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