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Mixed spin-charge solitons and thermodynamics of $(TMTTF)_2X$

SUMIT MAZUMDAR, University of Arizona, R. TORSTEN CLAY, R. P. HARDIKAR, Mississippi State University — The $(TMTTF)_2X$ salts are quasi-one-dimensional materials that undergo two phase transitions as the temperature is lowered from 300 K under ambient pressure. The high temperature transition at $T_{CO} \sim 100$ K is to a charge-ordered (CO) state. The low temperature transition is often to a spin-Peierls (SP) state that appears at $T_{SP} \sim 10$ K, and that competes with the CO state. We have investigated the thermodynamics of these systems within an extended Hubbard Hamiltonian that includes (a) on-site and nearest neighbor Coulomb interactions, and (b) bond- and site-coupled quantum phonons. From calculations of charge, bond and spin-susceptibilities we are able to explain the transition from the CO to the SP state. The CO state corresponds to the charge occupancy scheme ...1010... (where '1' and '0' denote charge-rich and charge-poor sites respectively), while the SP state has charge occupancy ...1100.... The transition from the CO to the SP phase as temperature is lowered is driven by spin effects: At high temperatures, high-spin states dominate the free energy, and favor the ...1010... CO configuration. At low temperatures, spin singlet states dominate the free energy and instead favor a singlet SP state with the ...1100... charge pattern. In the temperature region $T_{SP} < T < T_{CO}$ there occur mixed spin-charge solitons that are domain walls between the ...1010... and ...1100... charge patterns.

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