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Bond patterns in 1/4-filled spin-Peierls materials¹ ANDREW WARD, R. TORSTEN CLAY, Mississippi State University, NILADRI GOMES, SUMIT MAZUMDAR, University of Arizona — In the 1/4-filled quasi-one dimensional molecular charge transfer solids (CTS) there exist two distinct classes of spin-Peierls (SP) transitions. The two classes are distinguished by differing bond patterns: either the pattern Strong-Medium-Weak-Medium (SMWM), or the pattern Strong-Weak-Strong-Weak' (SWSW'). Experimentally the SP transition temperature of CTS of the first type (SMWM) is much higher than those of the second type (SWSW'). This indicates that the small change in bond patterns within the SP phase greatly affects the electronic behavior of the CTS. We show that these two bond patterns can be explained within the one dimensional Extended Hubbard Model. We use quantum Monte Carlo and finite-size scaling to create a phase diagram for the 1/4-filled 1D CTS and discuss charge order amplitude and other experimental observables.

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