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Numerical Study of Finite-Temperature Phase Transitions in Quasi-One-Dimensional Molecular Conductors YUICHI OTSUKA, CREST-JST, JAEA/SPring-8, HITOSHI SEO, JAEA/SPring-8, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo, TAKEO KATO, Institute for Solid State Physics, University of Tokyo — We have theoretically investigated the charge ordering, the dimer Mott, and the spin-Peierls phase transitions in quarter-filled quasi-one-dimensional organic conductors, such as $DCNQI_2X$ and $TMTTF_2X$, by considering the extended Hubbard model with electron-lattice couplings and inter-chain Coulomb interaction. We apply the stochastic-series-expansion quantum Monte Carlo method to the effective one-dimensional model obtained by the adiabatic and inter-chain mean-field approximation. Temperature dependences of the order parameters and the susceptibilities are calculated for the charge ordering, the dimer Mott, and the spin-Peierls transitions. The results show a competition between the charge-ordered and dimer Mott insulating states, consistent with our previous work [1], and both of them undergo the spin-Peierls transition at low temperatures. There, two types of spin-Peierls phases with spin gap appear in competition with showing different orderings of period four in lattice distortion and charge disproportionation. [1] H. Seo, Y. Motome, and T. Kato, J. Phys. Soc. Jpn. **76**, 013707 (2007).

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