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Charge frustration and novel electron-lattice coupled phase transition in organic conductor DI-DCNQI₂Ag HITOSHI SEO, JAEA/SPring-8, YUKITOSHI MOTOME, Department of Applied Physics, University of Tokyo — We have theoretically investigated the phase transition accompanying charge ordering in 1/4-filled quasi-one-dimensional organic conductor DI-DCNQI₂Ag. The nature of this phase transition at 220 K has been under debate since the first direct observation of charge ordering among organic conductors by Hiraki and Kanoda[1]. In this study, motivated by a recent synchrotron radiation x-ray study by Kakiuchi *et al.*[2], we investigate a three-dimensional interacting spinless fermion model coupled to the lattice degree of freedom. We have found that the peculiar "spiral frustration" existing in the interchain Coulomb interaction destabilizes simple Wigner crystal-type charge order and gives rise to a novel state where different chains show different orders and align periodically: charge order, lattice dimerization, and a co-existence of them. The co-existence of these two orders was in fact predicted in our previous study for the non-frustrated case[3], which was stabilized as a result of competing interactions. In contrast, the co-existence in the present study is obtained by compromising the frustration in charge sector. [1] K. Hiraki and K. Kanoda, Phys. Rev. Lett. 80 (1998) 4737. [2] T. Kakiuchi et al., Phys. Rev. Lett. 98 (2007) 066402. [3] H. Seo, Y. Motome, and T. Kato, J. Phys. Soc. Jpn. 76 (2007) 013707.

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