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Spin frustration and charge ordering in TMTTF salts
KAZUYOSHI YOSHIMI, NRI "RICS," AIST, Department of Physics, University of Tokyo, HITOSHI SEO, Advanced Science Institute, RIKEN, CREST JST, SHOJI ISHIBASHI, NRI "RICS," AIST, STUART BROWN, Department of Physics and Astronomy, UCLA — Quasi-one-dimensional organic conductors $(TMTTF)_2X$ salts exhibit various types of phase transitions such as magnetic ordering, charge ordering (CO), and superconducting transitions. Among them, $(TMTTF)_2SbF_6$ shows a peculiar behavior under pressure: a cooperative reduction of CO and antiferromagnetic (AF) phase transition temperatures by the application of pressure has been reported by NMR measurements [1]. This result naively does not coincide with the case for typical CO transitions, where CO suppresses the tendency toward magnetic ordering due to decrease of the effective spin exchange coupling. To explain this behavior, we investigate a 1/4-filled quasi-one-dimensional extended Hubbard model with Coulomb interactions and inter-chain hopping which causes spin frustration between the dimers on the one-dimensional chains. By numerical exact diagonalization method, we find that CO relaxes spin frustration and enhances two-dimensionality which stabilizes AF ordering. To compare our results with experiments, we determine the hopping parameters by first principles band calculation for several TMTTF salts and discuss the relation between spin frustration and CO.
[1] W. Yu et al., Phys. Rev. B. 70 121101 (2004).

Kazuyoshi Yoshimi
NRI "RICS," AIST, Department of Physics, University of Tokyo

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