Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Tuning the magnetic dimensionality by charge ordering in the molecular TMTTF salts KAZUYOSHI YOSHIMI, Department of Physics, University of Tokyo, Nanosystem Research Institute "RICS", AIST, HITOSHI SEO, Condensed Matter Theory Laboratory, RIKEN, SHOJI ISHIBASHI, Nanosystem Research Institute "RICS", AIST, STUART BROWN, Department of Physics and Astronomy, UCLA — Low-dimensional (D) organic conductors $TMTTF_2X$ are considered as a prototypical system for investigations of D-crossover phenomena, since the transfer integrals connecting the conduction chains are readily controlled by applied pressure [1]. In addition, recent NMR experiments in TMTTF salts imply the existence of another type of D-crossover which accompanies a multiferroic property; decreasing the ferroelectric-type charge ordering (FCO) by pressure is associated with the suppression of the antiferromagnetic (AF) transition temperature [2]. In this work, we theoretically investigate the interplay between FCO and magnetic states in TMTTF salts [3], and show that FCO increases 2-D AF spin correlation, whereas in the 1-D regime two different spin-Peierls states are stabilized. By performing first-principles band calculations for different salts and comparing our results with experiments, we identify the controlling parameters in the experimental phase diagram to be not only the inter-chain transfer integrals but also the amplitude of the FCO. [1] D. Jerome, Science 252, 1509 (1991). [2] W. Yu *et al.,* Phys. Rev. B. **70** 121101 (2004). [3] K. Yoshimi, H. Seo, S. Ishibashi, and S. E. Brown, arXiv:1110.3573 and arXiv:1110.3575.

Kazuyoshi Yoshimi
Department of Physics, University of Tokyo,
Nanosystem Research Institute "RICS", AIST

Date submitted: 27 Nov 2011 Electronic form version 1.4