Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Effective model and spin/charge ordering in molecular conductors X[Pd(dmit)$_2$]$_2$ HITOSHI SEO, RIKEN/JST-CREST, TAKAO TSUMURAYA, RIKEN/National Institute for Materials Science, MASAHISA TSUCHIIZU, Nagoya University, TSUYOSHI MIYAZAKI, National Institute for Materials Science, REIZO KATO, RIKEN — The family of molecular conductors, β'-type X[Pd(dmit)$_2$]$_2$ (X: monovalent cation) salts, show a variety of electronic states: dimer-type Mott insulator, magnetic order, spin-liquid behavior, metallic/superconducting states, and a peculiar charge ordering involving multi-orbitals[1]. In this work, we construct an effective low-energy model which takes into account the multi-orbital degree of freedom. We consider fragments of molecular orbital as a basis set, nearly localized on either one of the dmit ligands. The transfer integrals are obtained for a series of salts by fitting to the first-principles band calculations[2]. We find that all the intra-dimer transfer integrals including the diagonal ones are of the same order; this results in a modification of the orbital scheme in strongly dimerized [Pd(dmit)$_2$]$_2$ discussed in the literatures, then to the effective one-band model. We calculate possible spin and charge ordering based on mean-field approximation to the extended Hubbard model incorporating the fitted parameters. [1] R. Kato, Chem. Rev. 104 (2004) 5319; K. Kanoda and R. Kato, Annu. Rev. Condens. Matter Phys. 2 (2011) 167. [2] T. Miyazaki and T. Ohno, Phys. Rev. B 59 (1999) 5269; T. Tsumuraya, H. Seo, M. Tsuchiizu, R. Kato, and T. Miyazaki, in preparation.

Hitoshi Seo
RIKEN

Date submitted: 07 Nov 2012 Electronic form version 1.4