"Pudding Mold"-type Band as an Origin of Large Thermopower in τ-type Organic Conductors

Hirohito Aizawa[1], Kazuhiko Kuroki[1], Harukazu Yoshino[2], and Keizo Murata[2]
[1]*Department of Applied Physics and Chemistry, The University of Electro-Communications, Japan*
[2]*Department of Molecular Materials Science, Graduate School of Science, Osaka City University, Japan*
Email: kuroki@vivace.e-one.uec.ac.jp

Recently, large thermopower has been observed in two-dimensional τ-type organic conductor τ-(EDO- *S*,*S*-DMEDT-TTF)$_2$(AuBr$_2$)$_{1+y}$. [1] The controllability of the band-filling [2] is a unique feature of this series of materials as contrasted to many organic conductors. Band structure calculated by using extended Hückel method has shown characteristic features such as the star-shaped Fermi surface around the Γ-point and a small energy gap that separates the upper and the lower flat portions of the band. [3]

Here, we calculate the electronic band structure for τ-(EDO-*S*,*S*-DMEDT-TTF)$_2$AuBr$_2$ and τ-(P-*S*,*S*-DMEDT-TTF)$_2$AuBr$_2$ using the linearized augmented plane wave (LAPW) method.[4] We obtain an effective tightbinding model by fitting the first principles band structure, in which we study the origin of the large thermopower using the Boltzmann's equation approach. The temperature dependence of the thermopower is in fair agreement with the experiments in both materials. We identify the origin of the large thermopower as the "pudding mold"-type band, which has been proposed as an origin of the large thermopower in Na_xCoO_2 [5]. Here, the small energy gap that separates the bottom of the "upper pudding" and the top of the "lower pudding", along with the deviation of the band filling from half-filling, plays a crucial.

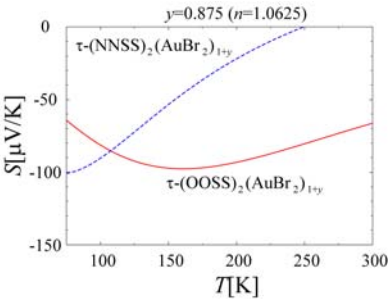

Fig. 1. Calculated Seebeck coefficient as functions of temperature for τ-(EDO-*S*,*S*-DMEDT-TTF)$_2$AuBr$_2$ (solid curve,OOSS) and τ-(P-*S*,*S*-DMEDT-TTF)$_2$AuBr$_2$ (dashed curve, NNSS) with y=0.875 (n=1.0625).

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