Highest Recorded *ZT* of Molecular-based Organic Conductors

Harukazu Yoshino

Graduate School of Science, Osaka City University, Osaka 558-8585, Japan

We are exploring organic conductors showing high dimensionless thermoelectric figure of merit defined as $ZT = S^2T/\rho\kappa$, where S, ρ, κ and T are thermopower, electrical resistivity, thermal conductivity and absolute temperature, respectively. One advantage of organic materials to get high ZT is their low κ usually in the order of 1 W K^{-1} m^{-1}. A large group of molecular-based organic conductors are salts composed of organic donor molecules like TMTSF and BEDT-TTF (Fig. 1) and monovalent inorganic anions. Their electronic systems are quasi-one- or quasi-two-dimensional since energy bands are constructed by anisotropic overlap of molecular orbitals of donors. Among them we have been focusing on τ-type conductors that show relatively large $|S|$ of about 100 μV K^{-1} even in metallic or weakly semiconducting states. Figure 2 shows molecular packing within a conducting layer of τ-$(OOSS)_2(AuBr_2)_{1+y}$, ($y \leq 0.875$).

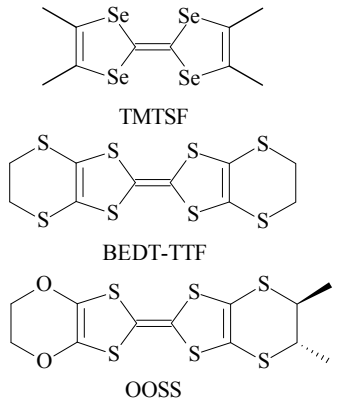

Fig. 1 Organic donor molecules giving organic conductors.

A difficulty to determine ZT of organic conductors is small size (~1 mm in length) and fragileness of their crystals. We have developed a system to determine ZT of such crystals by measuring ρ, S and κ simultaneously [1]. Up to now we have determined ZT of 8 kinds of τ-type conductors and the highest ZT is 0.068 (175 K) of τ-$(OOSS)_2(AuCl_2)_{1+y}$ (Fig. 3). This is also the highest of molecular-based organic conductors. The mechanism based on the pudding-mold type band model was proposed by Aizawa *et al.* to explain coexistence of large $|S|$ with metallic ρ [2].

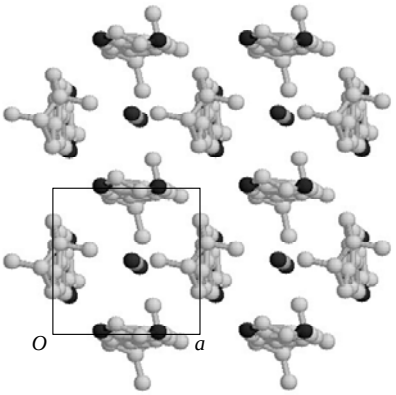

Fig. 2 Two-dimensional conducting layer of τ-$(OOSS)_2(AuBr_2)_{1+y}$, ($y \leq 0.875$).

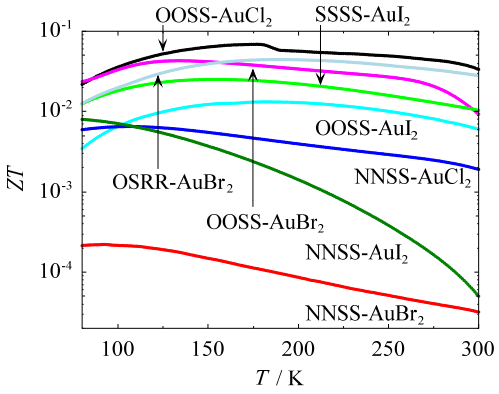

Fig. 3 Dimensionless thermoelectric figure of merit ZT of τ-type organic conductors.

[1] H. Yoshino *et al.*, J. Therm. Anal. Calorim. **92** (2008) 457.

[2] H. Aizawa *et al.*, Physica B **405** (2010) S27.