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Crystal Structures and Band Structures of Acene Chalcogenides: Their Application for OFET. A. UGAWA, T. KUNIKIYO, Y. OHTA, M. MURAKAMI, J. KASAHARA[1], Materials Labs., Sony Corp. — We have systematically studied acene chalcogenides as active channel materials for Organic Field Effect Transistor (OFET). The molecules have a common structural feature which is of great advantage for carrier channel: chalcogen atoms are located at outside of molecule so that larger orbitals of chalcogen atoms would intensify intermolecular interactions not only for the molecular stacking direction but also for the inter-stacking directions. We then expect that the conduction channels would become more isotropic and the effective mass of the carriers would become lighter compared to the case of aromatic hydrocarbons. The materials we have surveyed are as follows: Hexathiopentacene (HTP), Tetrathiotetracene (TTT), Hexathioanthracene (HTA), Tetrathioanthracene (TTA), Benzo[1,2-c;3,4-c';5,6-c"]tris[1,2]dithiole-1,4,7-trithione (abbreviated as C_9S_9, which is its chemical formula), and some selenium analogues. The first-principle band structure calculations based on the crystal structures determined by x-ray analysis reveal that the materials have an anisotropic 2-D HOMO band with an effective mass of $1.1m_e$ for TSeA, $1.3m_e$ for HTA, $1.4m_e$ for TTT, respectively. HTP is proved to have a 1-D HOMO band with m^*=$2.5m_e$ in spite of 2-D structural feature. It is interesting that C_9S_9 has an isotropic 3-D HOMO band with m^*=$0.68m_e$, properties which are suitable for OFET channel.

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