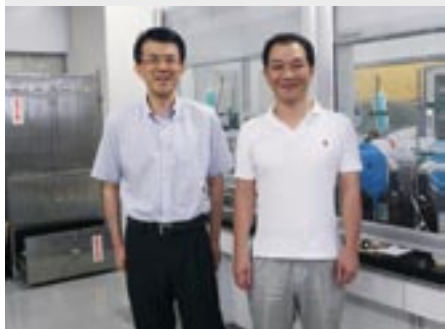


Development of Organic Semiconductors for Molecular Thin-Film Devices

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Organic light-emitting diodes (OLEDs) and organic field-effect transistors (OFETs) based on π -conjugated oligomers have been extensively studied as molecular thin-film devices. Organic semiconductors with low injection barriers and high mobilities are required for highly efficient OLEDs and OFETs. Radical cations or anions of an organic semiconductor have to be generated easily at the interface with an electrode (or a dielectric), and holes or electrons must move fast in the semiconducting layer. Compared with organic p-type semiconductors, organic n-type semiconductors for practical use are few and rather difficult to develop. Recently, we found that perfluorinated aromatic compounds are efficient n-type semiconductors for OLEDs and OFETs.

1. High-Mobility Bottom-Contact Thin-Film Transistor Based on Anthracene Oligomer¹⁾

The mobility in top- and bottom-contact thin-film transistors (TFTs) based on 2,2-bianthryl (**2A**) was improved. The mobility of the top-contact **2A**-TFT was improved from 0.25 to 1.0 cm²/Vs by octyltrichlorosilane (OTS) treatment of the SiO₂ gate-insulator surface. Large grains and clear step structures corresponding to the molecular length of **2A** were observed in the AFM image of a **2A** film deposited on the OTS-treated SiO₂. The bottom-contact **2A**-TFT with typical source-drain (S-D) electrodes of Cr/Au showed a non-linear rise in the output characteristics due to the large injection barrier

between the work function of Au and the HOMO level of **2A**. The non-linear rise in the output characteristics was successfully improved by employing MoO_x as the carrier injection layer for the S-D electrodes. Consequently, the mobility of the bottom-contact **2A**-TFT with a MoO_x/Au electrode was improved to 1.0 cm²/Vs, which is comparable to that in the top-contact **2A**-TFT.

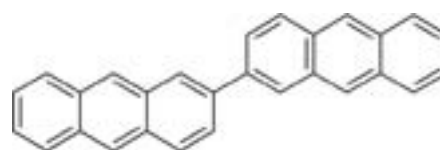


Figure 1. Structure of 2,2-bianthryl (**2A**).

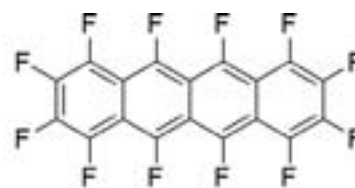
2. Structure, Morphology, and Growth Dynamics of Perfluoropentacene Thin Films²⁾

We report high structural order in thin films of the organic semiconductor perfluoropentacene (PFP), which is a candidate material for n-type applications, deposited by vacuum sublimation on oxidized silicon wafers. Bragg reflections up to high order in both specular and grazing incidence geometries and a mosaicity of less than 0.01° demonstrate the well defined structure. The thin film entirely consists of crystallites with a structure close to the bulk phase without any contamination with a second phase. Real-time X-ray measurements show that

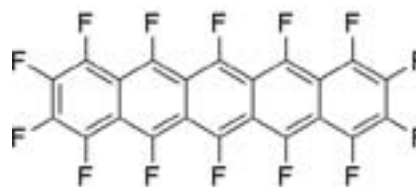
PFP grows in a Stranski–Krastanov growth mode with the first monolayer wetting the substrate before 3d-growth sets in during growth of the second monolayer. Implications for its use are discussed.

3. Impact of Perfluorination on the Charge-Transport Parameters of Oligoacene Crystals³⁾

The charge-transport parameters of the perfluoropentacene and perfluorotetracene crystals are studied with a joint experimental and theoretical approach that combines gas-phase ultraviolet photoelectron spectroscopy and density functional theory. To gain a better understanding of the role of perfluorination, the results for perfluoropentacene and perfluorotetracene are compared to those for their parent oligoacenes, that is, pentacene and tetracene. Perfluorination is calculated to increase the ionization potentials and electron affinities by ~1 eV, which is expected to reduce significantly the injection barrier for electrons in organic electronics devices. Perfluorination also leads to significant changes in the crystalline packing, which greatly affects the electronic properties of the crystals and their charge-transport characteristics. The calculations predict large conduction and valence bandwidths and low hole and electron effective masses in the perfluoroacene crystals, with the largest mobilities expected along the π -stacks. Perfluorination impacts as well both local and nonlocal vibrational couplings, whose strengths increase by a factor of about 2 with respect to the parent compounds.



Perfluorotetracene



Perfluoropentacene

Figure 2. Structures of perfluorotetracene and perfluoropentacene.

References

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