Temperature-dependent FET properties and charge transport capabilities of dibenzo[n]phenacenes (n = 5 -7)

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A new type of phenacene-based polycyclic aromatic molecules, dibenzo[n]phenacenes (**DBnP**s) (n = 5-7), were successfully synthesized, which are recognized as acene-phenacene hybrid molecules. The FET properties of single-crystal field-effect transistors (FETs) of **DBnP**s were systematically evaluated, demonstrating superior FET performance in **DB6P** to that of **DB5P** and **DB7P**,[1] *i.e.*, the higher field-effect mobility μ and ideal Shockley-type transfer curve. The FET performance would be largely influenced by extrinsic factors such as the formation of trap states between highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO), as well as intrinsic factors such as hopping (transfer) integrals between molecules in active layer.

In this work, the trap states generated at the interface between gate dielectrics and single crystal of **DBnP**s were quantitatively estimated from the temperature-dependent FET properties based on the multiple trap and release (MTR) model. Figure 1(a) shows the temperature-dependent μ values for **DBnP** single-crystal FETs. The intrinsic mobility μ_0 which refers to the μ value without any trap states was the highest for **DB6P,** and the ratio of the number of total trap states, N_t, with respect to that of valence states, N_v, was the smallest for **DB6P**. These results predict the highest FET performance for **DB6P FET.** The transfer integrals between adjacent molecules were calculated based on the molecular coordinates obtained by the single crystal X-ray diffraction of **DBnP**s, indicating that the transfer integrals were the largest for **DB6P** (Figure 1(b)), which also explains reasonably the excellent FET performance in the **DB6P** single-crystal FET. Thus, it has been found that the most significant factors dominating the transport characteristics in **DBnP** single-crystal FETs may be the closed molecular packing (or high transfer integrals) in the crystal lattice, in addition to the small trap density in **DB6P**.

1) Y. Zhang *et al.*, *Chem. Commun.*, **2021**, 57, 4768-4771.

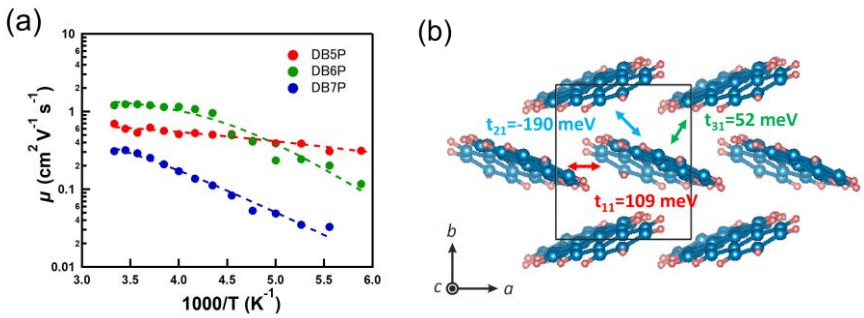

Figure 1. (a) Plots of μ *versus* 1000/*T* of **DBnP** single crystal FETs, together with the curves fitted with MTR model. (b) Transfer integrals between adjacent molecules of **DB6P**.