

An Unprecedented Ambipolar Charge Transport Material Exhibiting Balanced Electron and Hole Mobilities

Yuan-Li, Liao^a, Chi-Yen Lin^a, Yi-Hung Liu^a, Ken-Tsung Wong^{a*}, Wen-Yi Hung^{b*} and Wei-Jiun Chen^b

^a Department of Chemistry, National Taiwan University, Taipei, Taiwan 106. Fax: 886 2 33661667;

Tel: 886 2 33661665; E-mail: kenwong@ntu.edu.tw

^b Institute of Optoelectronic Sciences, National Taiwan Ocean University, Keelung, Taiwan 202.

E-mail: wenhung@mail.ntou.edu.tw

Electronic Supplementary Information

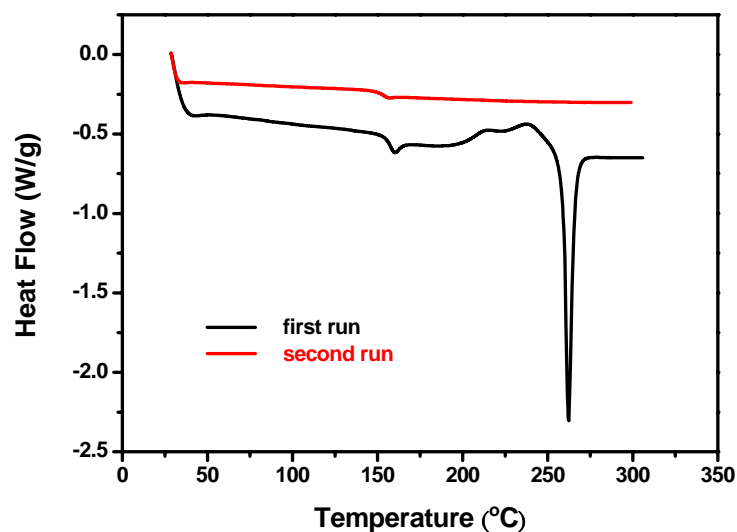


Fig. S-1: Differential scanning calorimetry (DSC) analyses of **27BPSF**. For the first run with heating rate of 20 °C/min., a glassy transition temperature (T_g) was found at around 160 °C and a distinct melting point (T_m) was detected at 262 °C. The isotropic sample then was quenched with liquid nitrogen to be a glassy solid which was heated in the second run with heating rate of 10 °C/min., the glassy transition temperature thus can be determined to be 150 °C, no further phase transition was detected after the T_g point.

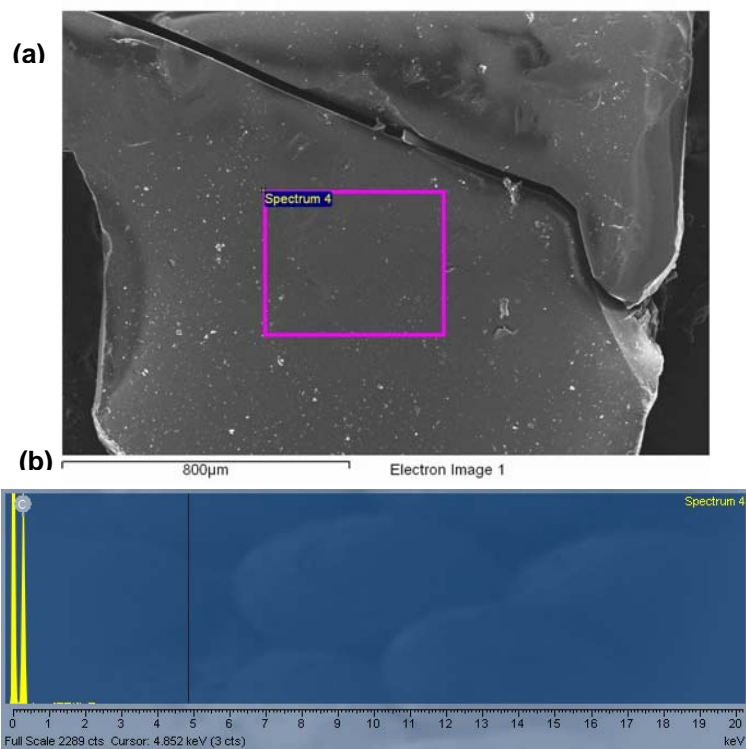


Fig. S-2: (a) The scanning electron microscope (SEM) image of a sublimed sample of **27BPSF**. (b) The energy dispersive X-ray (EDX) analysis spectrum of **27BPSF** detected within a specific area designated in a purple square in (a). The EDX spectrum clearly indicates that only carbon atom was detected, and no trace of Pd was found in the sample.

GDM analyses based on the field and temperature dependence of electron and hole mobilities.

The zero-field mobility $\mu(0,T) = \mu_0 \exp[-(2\sigma/3k_B T)^2]$ in equation 1 is obtained by extrapolation to zero field ($E = 0$) from results of Fig. 3. The semi-logarithmic plots of the zero-field mobilities versus $1/T^2$ for electrons and holes are shown in Figs. S-1(a). From the data, a linear relationship was observed with a transition at T_{ND} about 240 K for electrons and holes, which may be due to carriers not attaining dynamic equilibrium while migrating through the organic layer at low temperatures and thus becoming “dispersive”. For $T > T_{ND}$, the zero-field mobility values μ_0 , the energetic disorder width σ , and the degree of positional disorder Σ were determined. The prefactor mobilities (disorder-free mobilities) μ_0 for electrons and holes are about $7.4 \times 10^{-3} \text{ cm}^2/\text{V}\cdot\text{s}$ and $6.5 \times 10^{-3} \text{ cm}^2/\text{V}\cdot\text{s}$, respectively. It indicates that intrinsic intermolecular charge-transfer characteristics of **27BPSF** are similar capable of transporting electrons and holes. σ for electron and hole are about 69 meV and 65 meV, respectively. Inally, the slope $\beta(T) = C[(\sigma/k_B T)^2 - \Sigma^2]$ obtained from results of Fig. 3 was plotted versus $(\sigma/k_B T)^2$ for electrons and holes shown in Fig. S-1(b), and the values of C and Σ were determined. Σ for electrons and holes are 1.4 and 1.6, respectively. C for electrons and holes are $3.6 \times 10^{-4} \text{ V}^{1/2}/\text{cm}^{1/2}$ and $4 \times 10^{-4} \text{ V}^{1/2}/\text{cm}^{1/2}$, respectively.

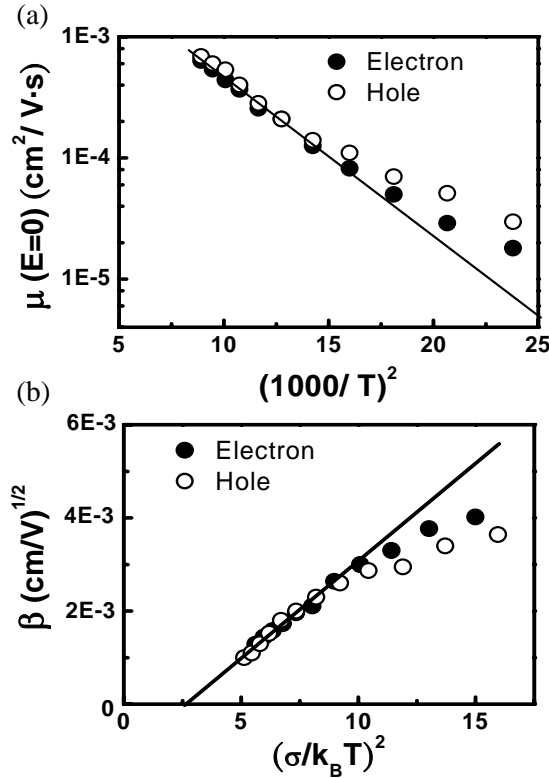


Fig. S-3: (a) Temperature dependence of mobilities at zero-field, (b) β vs. $(\sigma/k_B T)^2$ for **27BPSF**.

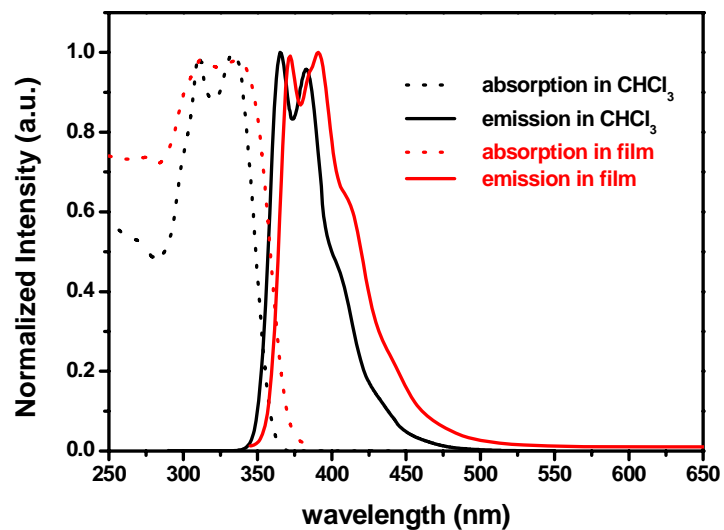


Fig. S-4: The electronic absorption and photoluminescence spectra of **27BPSF** in dilute CHCl_3 solution and in solid thin films. Both absorption and emission spectra of **27BPSF** were found to be slightly red-shifted as compared to those detected in solution, which are usual phenomena encountered in solid samples due to the different dielectric environments. Since there is no distinct low-energy peak was found in the spectra, we assume that there is no significant intermolecular interactions occurred in the amorphous thin films.