

ADVANCED FUNCTIONAL MATERIALS

Supporting Information

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Combinatorial Study of Temperature-Dependent
Nanostructure and Electrical Conduction of Polymer
Semiconductors: Even Bimodal Orientation Can Enhance 3D
Charge Transport

*Sangsik Park, Moo Hyung Lee, Kwang Seok Ahn, Hyun Ho
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Combinatorial Study of Temperature-Dependent Nanostructure and Electrical Conduction of Polymer Semiconductors: Even Bimodal Orientation Can Enhance 3D-Charge Transport

By Sangsik Park[#], Moo Hyung Lee[#], Kwang Seok Ahn[#], Hyun Ho Choi, Jihye Shin, Jie Xu, Jianguo Mei, Kilwon Cho, Zhenan Bao, Dong Ryeol Lee^{*}, Moon Sung Kang^{*} and Do Hwan Kim^{*}

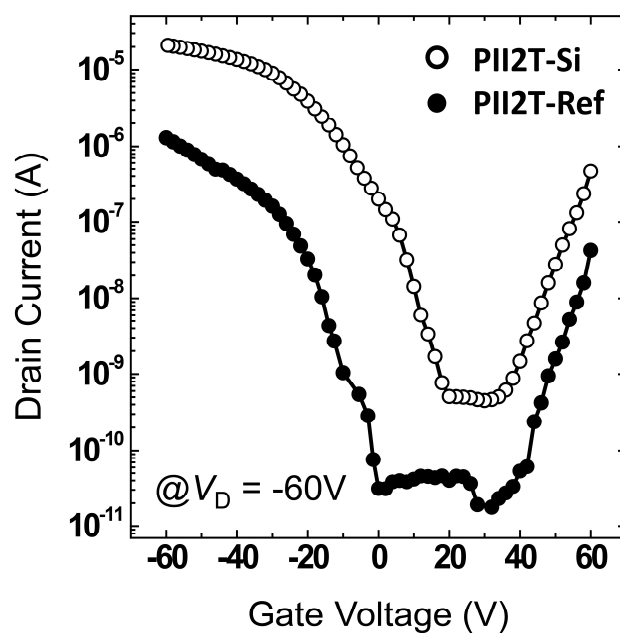


Figure S1. Transfer characteristic ($V_D = -60V$) collected at 300K for both the polymer FETs.

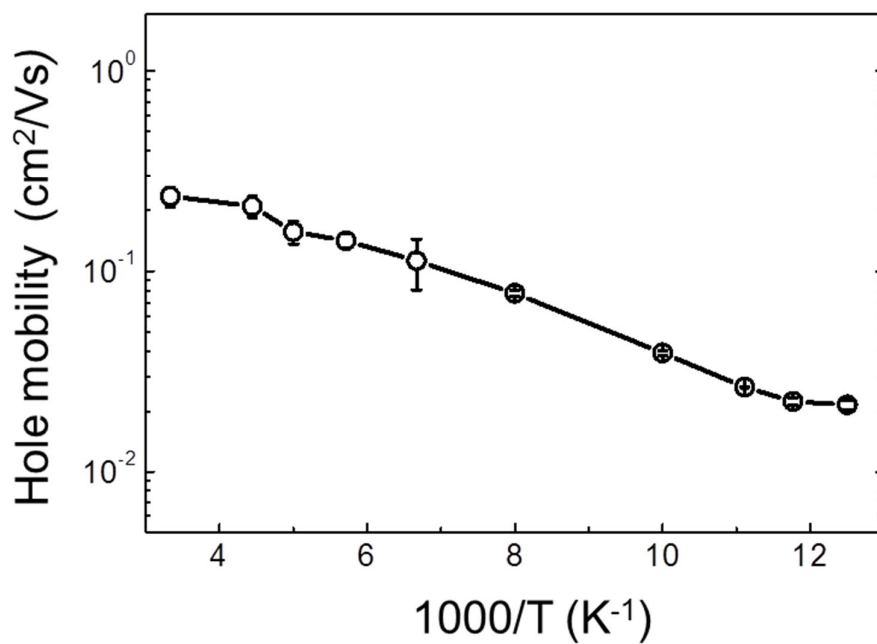


Figure S2. Arrhenius plot of the averaged hole mobility (μ) for the pentacene films. The mobilities were extracted from I_D vs. V_G characteristics measured at a constant V_D of -60 V.

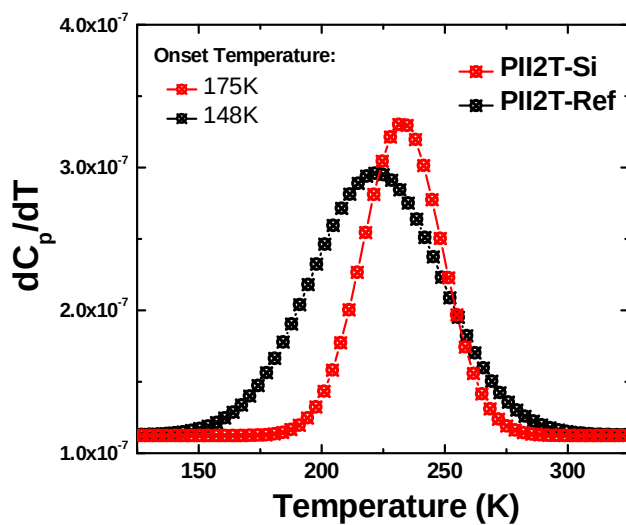


Figure S3. AC-chip calorimeter thermograms of the two polymer films, showing the derivative curve of the reversing specific heat capacity, dC_p/dT .

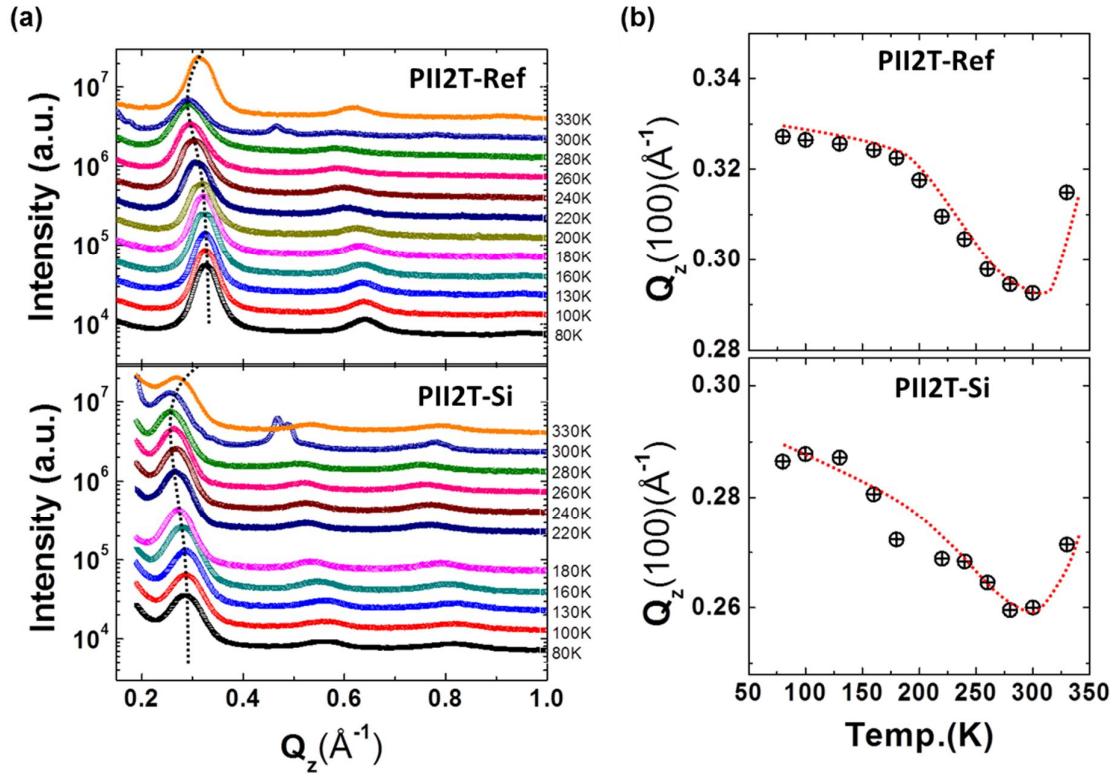


Figure S4. (a) Temperature-dependent on-specular X-ray diffraction profile (mode) and (b) lamellar d -spacing corresponding to (100) peaks for **PII2T-Ref** and **PII2T-Si** thin films

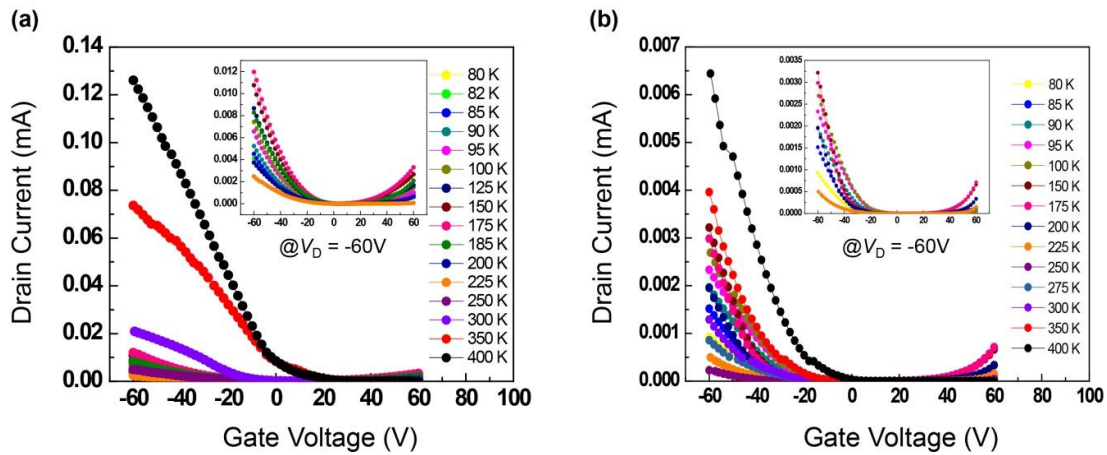


Figure S5. (a) Transfer characteristics ($V_D = -60V$) of a **PII2T-Si** thin film transistor collected at different temperatures. Inset : The enlarged view of the transfer characteristics (80K – 225K). (b) Transfer characteristics ($V_D = -60V$) of a **PII2T-Ref** thin film transistor collected at different temperatures. Inset : The enlarged view of the transfer characteristics (80K – 225K).

The 3-dimensional charge transport could be verified from a fitting method developed by Kronmeijer et al. [Adv. Mater. 2014, 26, 728] and Brondijk et al. [Phys. Rev. Lett. 2012, 109, 056601]. According to these reports, the channel current (I_D) between the source and drain electrodes in the saturation regime of an organic thin film transistor can be described by the following temperature (T) and voltage (V_G) dependence:

$$I_D^{2D} = A \frac{W}{L} d_{sc}^{1-\left(\frac{T_0}{T}\right)} \left(\frac{C_i}{e}\right)^{\frac{T_0}{T}} \frac{T}{T_0+T} (V_G - V_t)^{\left(\frac{T_0}{T}\right)+1} \text{ with } A = \sigma_0 \left(\frac{\frac{T_0^4}{T} \sin(\pi \frac{T}{T_0})}{8\alpha^3 B_c}\right)^{\frac{T_0}{T}} \quad (S1)$$

when 2-dimensional transport is assumed and

$$I_D^{3D} = \frac{A W}{e L} \left(\frac{1}{2K_b T_0 \epsilon_0 \epsilon_r}\right)^{\frac{T_0}{T}-1} C_i^{\frac{2T_0}{T}-1} \frac{T}{2T_0} \frac{T}{2T_0 - T} (V_G - V_t)^{\frac{2T_0}{T}} \quad (S2)$$

when 3-dimensional transport is assumed. Here, T_0 is the characteristic width of the exponential density of states, a^{-1} is the wavelength overlap localization length, s_0 is a conductivity prefactor, and B_c is the critical number for the onset of percolation. These equations can be simplified to power-laws such that $I_D \propto (V_G - V_t)^\gamma$ with $\gamma_{2D} = (T_0/T) + 1$ and $\gamma_{3D} = 2T_0/T$. Therefore, whether the transport takes place in 2-dimensional or in 3-dimensional can be determined from the plot between γ and $1/T$. Especially for 2-dimensional transport, the γ value would be extrapolated to 1 at infinite temperature (or at the y-intercept of the plot). For 3-dimensional transport, this value is extrapolated to 0.

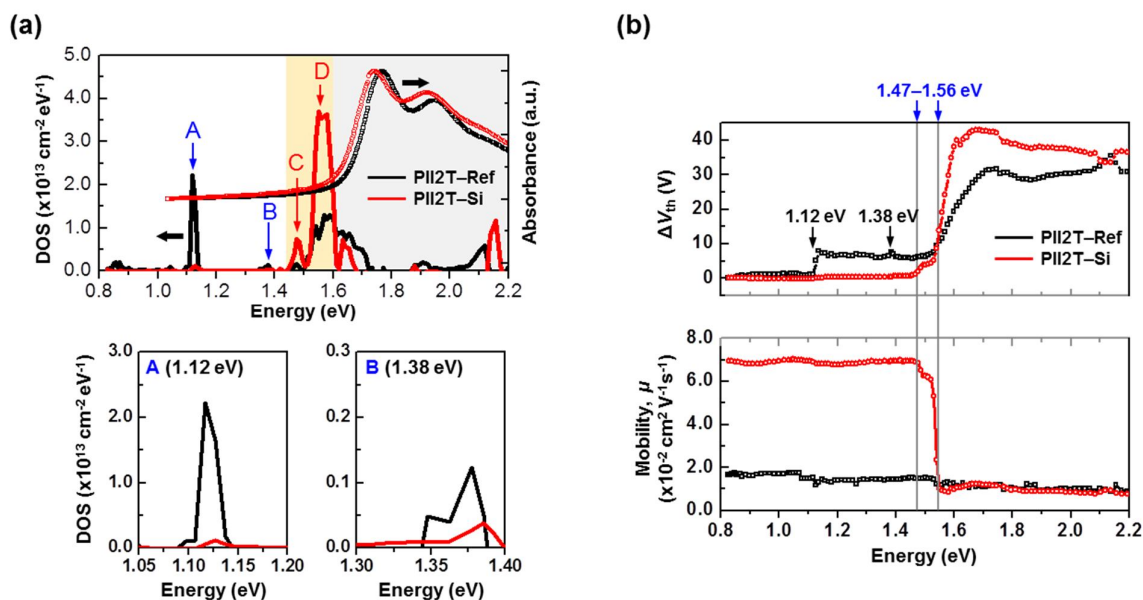


Figure S6. (a) The overall (up) and enlarged (down) DOS profiles for **PII2T-Ref** and **PII2T-Si** TFTs. The optical absorbance spectra of the polymer thin films are included together. (b) The dependence of threshold voltage shift (ΔV_{th}) and FET mobility on the energy of the incident photons.

Not only the distribution of the energy states near the transport level, the population of the **PII2T-Si** was found to be smaller than that of **PII2T-Ref** from photo-excited charge collection spectroscopy (PECCS) measurements.¹

(1) J. Lee, D. H. Kim, J.-Y. Kim, B. Yoo, J. W. Chung, J.-I. Park, B.-L. Lee, J. Y. Jung, J. S. Park, B. Koo, S. Im, J. W. Kim, B. Song, M.-H. Jung, J. E. Jang, Y. W. Jin, S.-Y. Lee, *Adv. Mater.* **2013**, 25, 5886.