

Electronic Supplementary Information

Assembly and Organization of Poly(3-hexylthiophene) Brushes and Their Potential Use as Novel Anode Buffer Layers for Organic Photovoltaics

José Alonzo,^a W. Michael Kochemba,^b Deanna L. Pickel,^c Muruganathan Ramanathan,^c Zhenzhong Sun,^d Dawen Li,^d Jihua Chen,^c Bobby G. Sumpter,^{c,e} William T. Heller,^a and S. Michael Kilbey II^{b,*}

^aBiology and Soft Matter Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831;

^bDepartments of Chemistry and of Chemical and Biomolecular Engineering, University of Tennessee, Knoxville, TN 37996;

^cCenter for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831;

^dDepartment of Electrical and Computer Engineering and Center for Materials for Information Technology, University of Alabama, Tuscaloosa, AL 35487;

^eComputer Science and Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831.

Thermal Characterizations. The temperature range used for studies of P3HT brush formation was identified through standard thermal gravimetric analysis performed using a TA Instruments Q5000IR TGA and a protocol in which the samples were heated from ambient temperature to 500.0 °C at 10.0 °C/min. Both P3HT-3K and P3HT-4K show an onset of degradation around 450 °C, as seen in **Figure S1**.

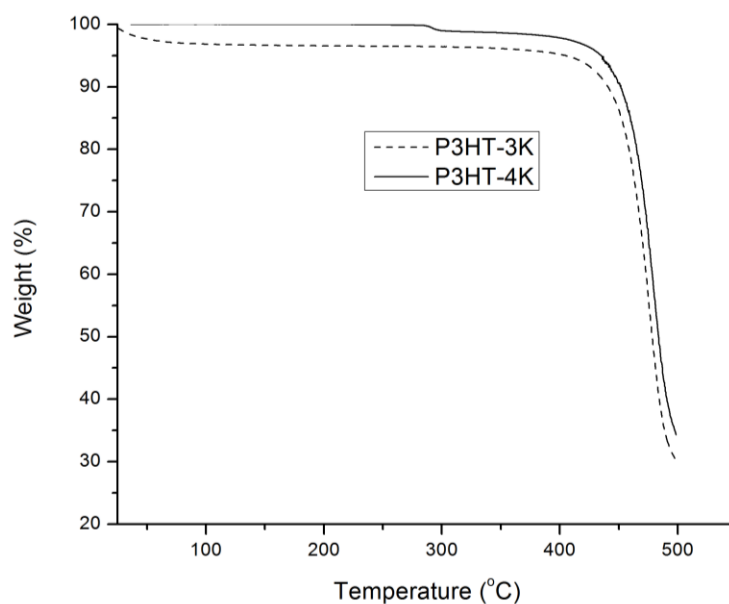


Figure S1. TGA thermograms of P3HTs used in this study.

A TA Instruments Q1000 differential scanning calorimeter (DSC) was used to evaluate thermal transitions of the P3HTs from the second heating ramp of a heat/cool/heat protocol. The DSC was baseline calibrated using sapphire standards (TA Instruments) and the temperature calibration was performed with an indium standard (melting point of 156.6 °C, provided by TA Instruments). Samples were first equilibrated at -50.0 °C, then heated to 250.0 °C using a ramp rate of 5.0 °C/min, cooled to -50.0 °C at 5.0 °C/min, and finally heated to 250.0 °C at the same ramp rate. Melting temperatures of 216 °C and 208 °C for P3HT-3K and P3HT-4K, respectively, are assigned from the peak in the heat flow curve acquired during a second heating cycle (identified by red crosses). **Figure S2** shows those DSC heat flow curves along with an inset plot showing the derivative of heat flow as a function of temperature. This representation of the data also indicates that melting temperatures are ~210 °C for these low molecular weight P3HTs. These melting temperatures are in good agreement with values reported by Zhao et al.^[S1]

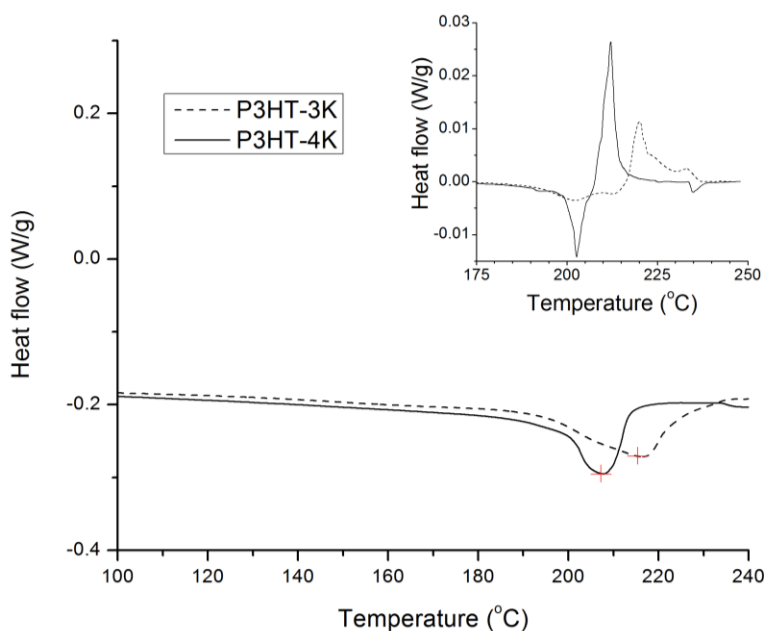


Figure S2. DSC heat flow traces of the second heating cycle and (inset) the derivative of heat flow.

Reference

- [S1] Zhao, J.; Swinnen, A.; Van Assche, G.; Manca, J.; Vanderzande, D.; Van Mele, B. J. *Phys. Chem. B* 2009, 113, 1587-1591.