Abstract Submitted for the MAR13 Meeting of The American Physical Society

Determination of the Crystallinity of Semicrystalline Poly(3hexyl thiophene) by Means of Wide Angle X-Ray Scattering JENS BALKO, Martin Luther University Halle-Wittenberg, Halle, Germany, RUTH LOHWASSER, MUKUNDAN THELAKKAT, University of Bayreuth, Germany, MICHAEL SOMMER, University of Freiburg, Germany, OVIDIU PASCUI, KAY SAALWAECHTER, THOMAS THURN-ALBRECHT, Martin Luther University Halle-Wittenberg, Germany — Poly(3-hexyl thiophene) (P3HT) is a common polymer semiconductor, often used as material or component in organic field effect transistors or solar cells. The crystallinity of this semicrystalline material is among other parameters governing the electronic mobility. However, at present there is no routine method available to determine an absolute value for the crystallinity, and the values given in the literature e.g. for the enthalpy of melting vary by a factor of three. Wide Angle X-Ray Scattering (WAXS) probes the crystals as well the amorphous parts of the sample. We present an approach for the determination of the crystallinity based on the evaluation of WAXS intensities at low scattering vectors emanating from the amorphous regions. The result is used for a calibration of the melting enthalpy (34 J/g) that can serve as a reference value for more convenient calorimetric techniques and compared to the results of recent NMR investigations. We discuss the crystallinity for a number of chemically well-defined samples, with different molecular weight and a typical commercial sample with broad molecular weight distribution. Despite the high crystallinities of 60 to 80% the crystallites exhibit a large amount of disorder.

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Date submitted: 08 Nov 2012

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