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Temperature Dependent Study of Regioregular and Regiorandom Poly (3-hexyl thiophene)s XIAOBO SHEN, THOMAS RUSSELL, University of Massachusetts Amherst — Structure evolution of bulk regioregular (rr) and regiorandom (rra) poly (3-hexyl thiophene)s (P3HT) with temperature has been characterized by wide angle X-ray diffraction (WAXD). Different thermal behaviors associated with the inter- and intra-molecular packing were shown as regioregularity changes. Transition temperature of $\sim 100^o$C for crystalline rr-P3HT has been assigned to side chain melting point where the thermal expansion along the edge-on direction shows a turning point separating solid and molten hexyl side chains. Meanwhile, $\pi - \pi$ stacking distance was observed to initially decrease and then increase upon heating, with a minimum at $\sim 100^o$C. The average inter-molecular distance of rra-P3HT was independent of temperature while the average intra-molecular distance increased upon heating. Molten rr-P3HT and rra-P3HT show same inter- and intra-molecular distance. Temperature UV-Vis absorption and photovoltaic device performance were also measured.

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