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Tuning Rod-Rod Interactions in Poly(3-alkylthiophene) Derivatives BRYAN BOUDOURIS, VICTOR HO, RACHEL SEGALMAN, University of California, Berkeley — Poly(3-alkylthiophene) (P3AT) derivatives are used commonly in polymer semiconducting applications. However, during the coating of P3AT thin films strong intermolecular interactions generally lead to the formation of semiconducting fibers. This prevents the formation of long-range ordered domains and complicates analysis of structure-property relationships in P3AT-containing devices (e.g., organic photovoltaic cells). Here, we show rod-rod interactions can be controlled by rational polythiophene side chain design. The effects of side chain passivation are evidenced by a depressed melting temperature and the presence of a liquid crystalline region. We show also that while the rod-rod interactions are lowered significantly in a polythiophene derivative with a branched side chain relative to straight chain P3ATs, the optoelectronic properties remain approximately constant. Importantly, this reduced melting temperature allows for the real-time evolution of a P3AT crystal structure at room temperature to be monitored on an experimentally convenient time scale. These structural data correlate well with field-effect charge carrier mobility measurements and provide a path for studying the mechanism of ordering in plastic electronics.

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