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Effects of chain stiffness on the performance of conjugated polymers WENLIN ZHANG, ENRIQUE GOMEZ, SCOTT MILNER, Pennsylvania State University — Conjugated polymers, though still outperformed by their inorganic counterparts, are promising materials for flexible electronics, including field-effect transistors and solar cells. In order to design new materials and optimize existing polymers, we want to establish concrete links between chain properties, structural order, and electronic properties. Here we emphasize that a fundamental chain parameter, the persistence length, which characterizes the bending stiffness of chain backbones, is critical to the performance of conjugated polymers. The backbone stiffness affects not only chain conformations, but also configurational order for semiflexible chains. Using molecular dynamics simulations and analytical theories, we demonstrate that chain stiffness, together with the nematic interactions between backbone moieties, governs nematic phase behaviors and molecular packing at interfaces for conjugated polymers. The structural order, as a function of chain stiffness, in turn enhances charge transport. Because we can efficiently predict persistence lengths, liquid crystallinity, and interfacial ordering based on chemical structures, our overall work can help screen novel semiconducting polymers for high performance electronic devices.

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