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A Computational Investigation of the Structure and Optical Properties of Nanoconfined Semiconducting Polymers M.L. DRUMMOND, B.G. SUMPTER, Oak Ridge National Laboratory, M.D. BARNES, University of Massachusetts, Amherst, W.A. SHELTON, JR., R.J. HARRISON, Oak Ridge National Laboratory — The promise of semiconducting organic polymers lies in their incredible flexibility, both through varied structure types and via chemical modifications of the polymer backbone. One type of structure we have recently explored, both experimentally and theoretically, arises from the use of ink-jet printing methods to produce nanoconfined particles with arbitrary size and composition. We have found substantial evidence indicating the production of highly ordered, rod-shaped, pi-stacked folded chain structures for single molecule PPV-based systems. Results show that chain organization, which is greatly influenced by the solvent, is crucial in determining the photophysical properties. Recent multiscale calculations, including molecular dynamics, molecular mechanics, and both ground-state and excited-state ab initio calculations, have been used to elucidate the role of the substituents in controlling the structure of the nanoconfined polymer, as well as the resultant effect on the optical properties. Through this work, a structure-property relationship is developed that will prove to be of great utility to experimentalists and polymer theorists alike.

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