This work reports a comprehensive investigation of the effects of the processing additive diiodooctane (DIO) on the morphology of the established blend of PBDTTT-C-T polymer and the fullerene derivative PC71BM used in organic photovoltaics (OPVs), starting from the casting solution and tracing the effects to spun-cast thin films by using neutron/x-ray scattering, neutron reflectometry and other characterization techniques corroborated by theory and modeling. The results reveal that DIO has no observable effect on the structures of PBDTTT-C-T and PC71BM in solution, however in the spun-cast films, it significantly promotes their molecular ordering and phase segregation, resulting in improved power conversion efficiency (PCE). Thermodynamic analysis based on Flory-Huggins theory provides a rationale for the effects of DIO on different characteristics of phase segregation due to changes in concentration resulting from evaporation of the solvent and additive during film formation. In summary, a comprehensive suite of characterization techniques and theoretical analyses revealed both the lateral and vertical morphological effects of the processing additive diiodooctane, DIO, on the formation of bulk-heterojunctions and the resulting organic photovoltaic device parameters starting from a donor/acceptor polymer blend PBDTTT-C-T:PC71BM in solution, to the spin-cast films.

Reference
“Understanding how processing additives tune the nanoscale morphology of high efficiency organic photovoltaic blends: From casting solution to spun-cast thin film” Ming Shao,1, 1 Jong Kahk Keum,1, 1, 1 Rajeev Kumar1, 1, 1, Jihua Chen,1 James F. Browning,2 Sanjib Das,4 Wei Chen,5 Jianhui Hou,6 Changwoo Do,2 Kenneth C. Littrell,2 Adam Rondinone,1 David B. Geohegan,1 Bobby G. Sumpter,1 and Kai Xiao1
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