Supporting Information

Conformation-Dictated Aggregation Photophysics in Isoindigo-Based Copolymers

Eninges Asmare,^{†,‡} Nika Bekri,^{¶,§,∥} Leonato Tambua Nchinda,[⊥] Fekadu Gashaw,[†] Wendimagegn Mammo,[#] Tjaart P. J. Krüger,^{⊥,@} and Newayemedhin A. Tegegne *,[†]

†Department of Physics, Addis Ababa University, 1176 Addis Ababa, Ethiopia, ‡Department of Physics, Wollo University, Dessie, Ethiopia., ¶Department of Mathematics, Physics and Statistics, Addis Ababa Science and Technology University, 16417, Addis Ababa, Ethiopia., §Sustainable Energy Center of Excellence, Addis Ababa Science and Technology University, 16417, Addis Ababa, Ethiopia., ¶Nano Technology Center of Excellence, Addis Ababa Science and Technology University, 16417, Addis Ababa, Ethiopia., †University of Pretoria, Department of Physics, Pretoria, South Africa., †Department of Chemistry, Addis Ababa University, 33658, Addis Ababa, Ethiopia. @National Institute for Theoretical and Computational Sciences, (NITheCS), South Africa.

E-mail: newaye.medhin@aau.edu.et

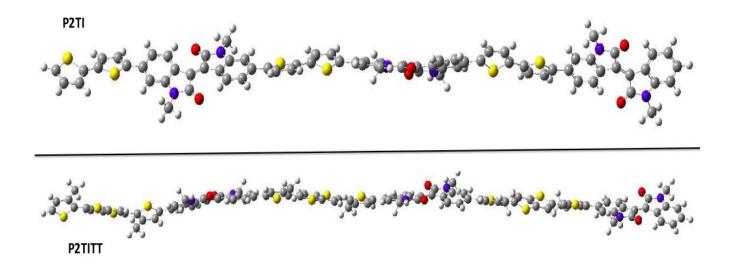


Figure S1: Side view of optimized geometries for trimetric units of P2TI (top) and P2TITT (bottom)

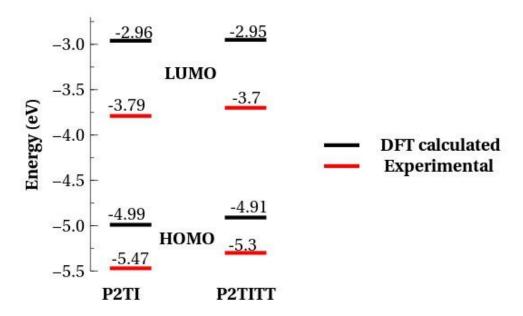


Figure S2: Comparison of the DFT-calculated and experimental HOMO-LUMO levels of P2TI and P2TITT.

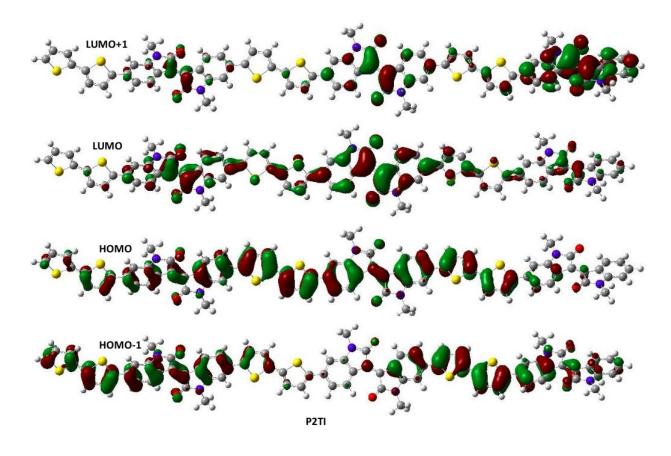


Figure S3: Electron cloud distribution in frontier molecular orbitals of P2TI.

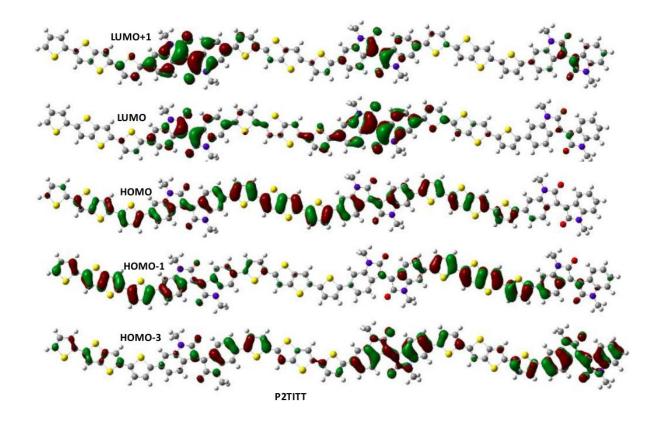


Figure S4: Electron cloud distribution in frontier molecular orbitals of P2TITT.

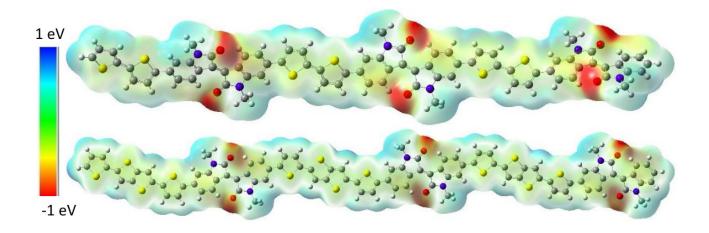


Figure S5: Electrostatic potentials surface in trimeric units of P2TI (top) and P2TITT (bottom).