Characterization of PMeT thin films for solar cell applications: An experimental and theoretical analysis

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PMeT films doped with Lithium tetrafluoroborate were deposited on tin oxide coated glass and stainless steel substrates using electropolymerization technique. It is found that galvanostatic method is more suitable for the electropolymerization of PMeT on conducting glass or flexible metal surfaces. Homogeneous films of PMeT could be deposited for the 3.0 – 1.0 mA/cm^2 constant current densities and for any dopant concentration in between 0.1M-0.2M range. However, the homogeneous and thick films could be grown only with 2.1 mA/cm^2 current density and 0.1M dopant concentration. The films were characterized using SEM, AFM, XRD, FTIR, Raman and UV-Vis absorption techniques. Raman and FTIR spectra of the samples revealed no signal related to the dopant, indicating that the optimum dopant concentration was well below the threshold value. The dopant incorporated into the PMeT films form highly confined conjugational defects, neither dynamically nor electronically coupled with the host lattice. Highly semi conductive PMeT thin films could be prepared by 0.1M doping of Lithium tetrafluoroborate. Theoretical calculations based on the density function theory (DFT) are used to explain the structural influence of the polymer and Li dopant concentration to its band gap and electronic structure. These calculations determine the optimum geometrical configurations of the *cis* and *trans* polymers and their corresponding electronic structures and demonstrate how the control of these parameters can lead to the production of a polymer of particular band gap, suitable for particular device application.

TOPICS + KEYWORDS: Solar Cells, polymer, PMeT, Cis-Trans, DFT, *Molecular simulation*.