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3-Hexyl-2,5-diphenylthiophene:phenylene vinylene-based conjugated polymer for solar cells application

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3-Hexyl-2,5-diphenylthiophene:phenylene vinylene-based conjugated polymer for solar cells application.

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Abstract A conjugated polymer, poly(3-hexyl-2,5-diphenylthiophene)-p-bisdodecyloxy-phenylene vinylene) (**CP**) was synthesized whose chemical structure was confirmed by 1 H-NMR and FTIR. **CP** possesses electrochemical band gap of 2.19 eV, determined by cyclic voltammetry (CV), and low laying highest occupied molecular orbital (HOMO) energy level (5.24 eV). Acting as an electron donor, **CP** was mixed with electron acceptor PC₆₁BM in (1:1, w/w) to fabricate the photoactive layer. The resultant **CP**:PC₆₁BM (1:1, w/w) based polymer solar cell (PSC) under AM 1.5G (100 mWcm⁻²) showed power conversion efficiency (PCE) of 2.66% with an open-circuit voltage (V_{OC}) of 678 mV, a short circuit current density (J_{SC}) of 7.711 mA/cm² and a fill factor (FF) of 50%. Band gap of **CP** calculated by Density functional theory (DFT) measurement was determined to 2.04 eV, which was in good agreement with the experimental value obtained by CV.

Keywords Conjugated polymer, photoactive solar cell, open-circuit voltage, density functional theory

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