

Effect of Poly (3-Hexylthiophene): Mixed Fullerene Indene-C₆₀ Multi-Adducts Ratios on the Performance of Organic Solar Cells

Hassan Tarikhum B.^{1,2}, Basil Ali¹, Furqan Almyahi^{1,*}, Mazin A. Mahdi¹

* furqan.kasim@uobasrah.edu.iq

¹ Department of Physics, College of Science, University of Basrah, Basrah, Iraq

² Department of Physics, College of Science, University Al Muthanna, Al Samawa, Iraq

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Abstract: In this study, poly (3-hexylthiophene) (P3HT) and fullerene Indene-C₆₀ multi-adducts (IC_xA) were blended to create a formulation as a solution and thin films, which were prepared under ambient conditions. The optical properties of various compositional ratios were studied using UV-Visible absorbance and photoluminescence (PL) measurements. The energy gaps of the prepared thin films and solutions were determined, and their values increased with increasing fullerene ratio because of the isolation of P3HT chains from their neighbors. Intensity ratio ($I_c = I_{c-c}$) with a small value in addition to a low value of full width at high maximum (FWHM) of Raman spectra are associated with increased conformation and high aggregation of composition. Furthermore, according to X-ray diffraction (XRD) results the 1:0.8 and 1:0.6 ratios have the largest crystallite sizes in comparison to the other ratios. The highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) levels for blends by electrochemical measurements were determined, which are sandwiched between those of the pure materials. In ambient conditions, binary organic photovoltaic cells (OPVs) at different ratios of the photoactive layer were evaluated. The device with a ratio of 1:0.6 had the best performance, with power conversion efficiency (PCE) of 1.21%, open circuit voltage (V_{oc}) of 0.53 V, short circuit current density (J_{sc}) of 5.71 mA/cm², and fill factor (FF) of 39.5% at a small V_{loss} of 1.39 V.

Keywords: Organic photovoltaics, Photoluminescence, X-ray diffraction, Raman spectrum, Cyclic Voltammetry.

1. INTRODUCTION

Organic materials have contributed to the development of organic photovoltaic cells (OPVs) as a new source of clean and cheap energy and have opened the way to progress in understanding the fundamental chemistry and physics of π -bonded macromolecules [1]. The OPV devices can absorb sunlight and convert it into electricity because of their conjugated system [2]. The first OPV device was constructed by Calvin in 1958 [3] using magnesium phthalocyanines (MgPc) between two conducting glass electrodes, which achieved 200 mV. The photovoltaic properties of these cells depend strongly on the nature of the electrodes. These cells are called single-layer organic photovoltaic cells and are the simplest among various organic photovoltaic cells. The first organic photovoltaic cell bilayer was reported by Tang in 1986 [4]. In these devices, light is usually absorbed in the donor material (copper phthalocyanine) and the photogenerated excitons diffuse within the donor towards the planar interface to the acceptor material (perylene tetracarboxylic derivative). A power conversion efficiency of approximately

1% has been achieved under simulated AM2 illumination (light intensity of 75 mW/cm²). However, the performance of these devices is limited by the small interfacial area between the donor and acceptor materials, which results in impaired charge separation. To achieve high-performance OPV devices and to increase exciton dissociation in the donor/acceptor interfaces, an interpenetrated bulk heterojunction (BHJ) structure of the donor and acceptor should be achieved, which invented by Heeger et al. [5]. Blending an electron-donating conjugated polymer such as poly (3-hexylthiophene) (P3HT) with a fullerene electron acceptor such as [6, 6]-phenyl C₆₀ butyric acid methyl ester (PCBM) contributed to improving the morphology of the active layer, charge separation at the donor/acceptor interface, and transport between layers of solar cells [6]. PCBM was replaced by another fullerene derivative, indene-C₆₀ mono-adduct (ICBA), which has a higher LUMO than PCBM [7]. Indene: fullerene synthesized by the simple reflux of indene and fullerene, such as indene-C₆₀ mono-adduct (ICMA), indene-C₆₀ bis-adduct (ICBA), and indene-C₆₀ tris-adduct (ICTA), which is characterized by a lower cost