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كلية العلوم – قسم الكيمياء



Preparation and Evaluation of Overlapping Layers of
Carbon Allotropes, Metal-Halides, Conducting-
Polymers for Energy Applications

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ABSTRACT

One of the most key factors that impact the hybrid metal halides-organic perovskite solar cells (PSCs) are the chargers transport layers including holes and electrons transport layers; HTLs and ETLs respectively. The HTLs affect the PSCs and lead to the disparate performance of the same absorber layer due to the difference between the various utilized HTLs in hole mobility and electric conductivity. Carbon allotropes materials have arisen as a potential candidate due to their abundance, easy preparation, low cost, suitable electron band level, and outstanding stability. N-doped and N-functionalized graphene (N-DG and N-FG) derivatives are mostly promising materials; they are easy to prepare and employ for various applications. N-DG depends on doping the graphene structure with nitrogen atoms, while N-FG is mainly the meaning of grafting graphene surface covalently or non-covalently with a nitrogen compound. There are several methods to prepare N-DG, including wet chemical process, bombardment, and high thermal treatments methods. At the same time, N-FG is usually synthesized through a wet chemical reaction, including hydro and solvothermal techniques. **In the first part of this research**, three Nitrogen-functionalized graphene (NGs): amino-graphene (G-NH₂), graphene-ethanolamine (G-EA), and graphene ethylenediamine (G-EDA) have been synthesized and tested as hole transport layers (HTL) for perovskite solar cells (PSCs) applications. However, the fabricated device shows a very sufficient stable device, the PSCs fabricated with graphene-ethylenediamine (G-EDA) showed the best power conversion efficiency (PCE) of 12.85%. In order to overcome that dilemma, **in the second part of this research**, HTLs fabricated with bilayer structure engineering to synergy the stability and conductivity using graphene ethylene diamine (G-

EDA) as under layer and matching the valence band at HTLs: perovskite layer interface using conducting polymers (CPs) as a continuous contacted film to the absorber sunlight layer. Despite poly (3,4-ethylenedioxythiophene): poly (styrene sulfonate) (PEDOT: PSS) has been considered as the most successful CPs to use as an organic HTLs, it had been observed incomplete characteristics due to it has a high acidic value which influences the whole PSCs device. Photoluminescent test observed that at the optimum conditions of the deposited G-EDA/PEDOT: PSS obviously quenched the methylammonium lead iodide (MAPbI₃) emission perfectly than only PEDOT: PSS, which proved that G-EDA/PEDOT: PSS facilitated hole abstraction and transport from perovskite to the HTL. The champion PSCs device based on bilayer HTL structure gave power conversion efficiency (PCE) of 17.76% compared with 12.85 % for PEDOT: PSS-based PSCs.

Keywords:

Nitrogen-doped graphene; Nitrogen-functionalized graphene; Conductive polymers, Perovskite solar cells, Perovskite stability, Methylammonium lead iodide (MAPbI₃), Photoluminescent (PL), Time-resolved photoluminescent (TRPL), Power conversion efficiency (PCE), The Current density-voltage (*J-V*) characterization, Electrochemical impedance spectroscopy, Electrical equivalent circuit (EEC), Work function, Band gap, valence band incident photon-to-current conversion efficiency (IPCE), X-ray diffraction (XRD), Scanning electron microscopy (SEM), transmission electron microscopy (TEM), Ultraviolet-Visible (UV-Vis), Fourier transform infrared spectra (FTIR).

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