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Electrocatalytic and structural properties and computational calculation of PAN-EC-PC-TPAI-I_2 gel polymer electrolytes for dye sensitized solar cell application

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In this study, gel polymer electrolytes (GPEs) were prepared using polyacrylonitrile (PAN) polymer, ethylene carbonate (EC), propylene carbonate (PC) plasticizers and different compositions of tetrapropylammonium iodide (TPAI) salt. Linear sweep voltammetry (LSV) and electrochemical impedance spectroscopy (EIS) measurements were done using non-blocking Pt-electrode symmetric cells. The limiting current (J_{lim}), apparent diffusion coefficient of triiodide ions ($D^*_{I_3^-}$) and exchange current were found to be 12.76 mA cm^{-2}, 23.41 $\times$ 10^{-7} cm^2 s^{-1} and 11.22–14.24 mA cm^{-2}, respectively, for the GPE containing 30% TPAI. These values are the highest among the GPEs with different TPAI contents. To determine the ionic conductivity, the EIS technique was employed with blocking electrodes. The GPE containing 30% TPAI exhibited the lowest bulk impedance, R_b (22 Ω), highest ionic conductivity (3.62 $\times$ 10^{-3} S cm^{-1}) and lowest activation energy. Fourier transform infrared (FTIR) spectroscopy and X-ray diffraction (XRD) techniques were utilized for structural characterization. Functional group interactions among PAN, EC, PC and TPAI were studied in the FTIR spectra of the GPEs. An up-shift of the XRD peak indicates the polymer–salt interaction and possible complexation of the cation (TPA^+ ion) with the lone pair of electrons containing site –C≡N at the N atom in the host polymer matrix. On the other hand, computational study shows that TPAI-PAN based GPE possesses the lowest frontier orbital bandgap, which coincided with the enhanced electrochemical and electrocatalytic performance of GPE. The dye-sensitized solar cell (DSSC) fabricated with these GPEs showed that the J_{SC} (19.75 mA cm^{-2}) and V_{OC} (553.8 mV) were the highest among the GPEs and hence the highest efficiency, η (4.76%), was obtained for the same electrolytes.

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1. Introduction

One of the important components of dye-sensitized solar cells (DSSCs) is the electrolyte. The conducting polymers (CPs) have been regarded as alternative materials for DSSCs and other electronic devices because of their outstanding electrochemical properties, high electrical conductivity, high tensile strength, good stability and safety, ease of shaping, good processing ability, high flexibility, no spillage and low-costs.[1–7] Due to the outstanding benefits of CPs, various types of polymer electrolytes (PEs) have been studied for many years. Nowadays, there are diverse families of conventional polymer electrolytes, such as gel polymer electrolytes, ionic rubber forms of polymer electrolytes and polyelectrolytes.[8] There are a variety of traditional polymer based materials on or after synthetic polymers and their blends to biopolymer.[8] Some of the well known polymers are polyacrylonitrile (PAN),[9–12] polyethylene oxide (PEO),[13] polyethylene glycol (PEG),[14,15] poly(methyl

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