

Ionic liquid electrolytes based on 1-vinyl-3-alkylimidazolium iodides for dye-sensitized solar cells

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Abstract

Five new ionic liquids of 1-vinyl-3-alkylimidazolium iodide were synthesized to develop novel electrolytes for dye-sensitized solar cells. The effects of photovoltaic characteristics of the cell and the ionic liquid features such as viscosity and ionic conductivity were described. The 1-vinyl-3-alkylimidazolium cation volume was calculated by quantum chemistry method. The linear dependence of photon-to-current conversion efficiency on the non-solvated cation volume was revealed. After lithium iodide was added to 1-vinyl-3-alkylimidazolium salts as electrolytes, except the photovoltage, the photocurrent, fill factor and photon-to-current efficiency were improved correspondingly.

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1. Introduction

Dye-sensitized solar cells (DSSC) have attracted widespread scientific and technological interest owing to its high efficiency, reaching 10.6%, and as a low-cost alternative to traditional silicon solar cells [1]. The working principle of DSSC is based on ultrafast electron injection from a photoexcited dye into the conduction band of an oxide semiconductor and subsequent dye regeneration using electrolytes as hole transportation media. These electrolytes include conventional organic liquid electrolytes [2], solid-state p-type inorganic semiconductors [3], conductive organic materials [4], polymer electrolytes [5] and gel electrolytes [6]. However, some practical problems, such as long-term stability, may be serious obstacles in the process of using volatile organic liquid electrolytes. Recently, growing attention has been paid to room temperature

ionic liquids (RTIL), especially those with imidazolium salts and pyridinium salts, due to their favorable properties such as thermal stability, non-flammability, high ionic conductivity, negligible vapor pressure, and a possible wide electrochemical window [7]. This problem could be relieved by application of ionic liquids as electrolyte. Especially, 1-vinyl-3-alkylimidazolium salts have been prepared from the *N*-alkylation of 1-vinylimidazole with the corresponding alkyl halides. The polymers and gels were then synthesized by free-radical copolymerization of the 1-vinyl-3-alkylimidazolium halide and *N*-vinyl-2-pyrrolidone using azo-bis-isobutyronitrile as the initiator in methanol [8]. It is expected to introduce new electrolytic materials such as RTIL, gels and polymers for quasi-solid DSSC in the future [9,10].

In this work, 1-vinyl-3-alkylimidazolium iodide salts with different lengths of alkyl chain were prepared. We aim to describe the correlation between characteristics of ionic liquids and device photovoltaic performance and compare the ionic liquid electrolytes containing different lithium iodide quantities with regard to solar cell behavior.

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2. Experimental

2.1. Synthesis of ionic liquids

The 1-vinyl-3-alkylimidazolium iodide ionic liquids were synthesized from *N*-alkylation of 1-vinylimidazole with the corresponding alkyl iodide (Fig. 1) [11].

Under dry nitrogen atmosphere and vigorous stirring, 1.05 mol of freshly distilled alkyl iodide (RI, R = methyl, ethyl, *n*-propyl, *n*-butyl, *n*-amyl) was added dropwise over 2 h to 200 mL of 1,1,1-trichloroethane containing 1.0 mol of 1-vinylimidazole. After alkyl iodide drop addition was finished, the solution was kept refluxing for approximately 10 h until the two liquid phases formed clearly. The product was collected by the difference of polarity using a separatory funnel and washed with 1,1,1-trichloroethane to remove the unreacted reagents in the product. All the synthesized products are deep yellow liquids under room temperature. Their structures are confirmed by ¹HNMR (CDCl₃, δ/ppm relative to TMS, 500 MHz Bruker DRX500) as follows:

- 1-vinyl-3-methylimidazolium iodide (MVII):
10.53 (s, 1H), 7.92 (s, 1H), 7.75 (s, 1H), 7.47 (q, 1H, *J* = 8.4), 6.06 (q, 1H, *J* = 1.9), 5.48 (d, 1H, *J* = 6.3), 2.12 (s, 3H).
- 1-vinyl-3-ethylimidazolium iodide (EVII):
10.50 (s, 1H), 7.84 (s, 1H), 7.70 (s, 1H), 7.44 (q, 1H, *J* = 8.5), 6.04 (q, 1H, *J* = 2.0), 5.45 (d, 1H, *J* = 6.5), 4.54 (q, 2H, *J* = 6.5), 1.67 (t, 3H, *J* = 7.0).
- 1-vinyl-3-propylimidazolium iodide (PVII):
10.42 (s, 1H), 7.90 (s, 1H), 7.71 (s, 1H), 7.42 (q, 1H, *J* = 8.7), 6.03 (q, 1H, *J* = 2.5), 5.41 (q, 1H, *J* = 3.0), 4.40 (t, 2H, *J* = 7.0), 2.03 (t, 2H, *J* = 7.0), 0.99 (t, 3H, *J* = 7.5).
- 1-vinyl-3-butylimidazolium iodide (BVII):
10.29 (s, 1H), 7.89 (s, 1H), 7.67 (s, 1H), 7.34 (q, 1H, *J* = 8.5), 5.96 (q, 1H, *J* = 3.0), 5.31 (q, 1H, *J* = 2.5), 4.34 (t, 2H, *J* = 7.5), 1.86 (a, 2H, *J* = 7.5), 1.31 (h, 2H, *J* = 7.5), 0.85 (t, 3H, *J* = 7.5).
- 1-vinyl-3-amylimidazolium iodide (AVII):
10.33 (s, 1H), 7.67 (s, 1H), 7.60 (s, 1H), 7.36 (h, 1H, *J* = 9.0), 5.98 (q, 1H, *J* = 3.0), 5.33 (q, 1H, *J* = 3.0), 4.35 (t, 2H, *J* = 7.5), 1.90 (t, 2H, *J* = 7.5), 1.28 (t, 4H, *J* = 13.0), 0.79 (t, 3H, *J* = 6.5).

2.2. Computational methods

The frequency calculations of the successfully optimized 1-vinyl-3-alkylimidazolium structures reported here were

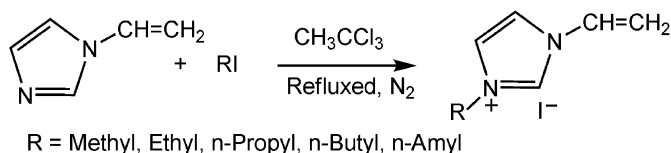


Fig. 1. Reaction of 1-vinyl-3-alkylimidazolium iodides formation.

performed with the Gaussian 98 program package on a Pentium IV PC. The 3–21G basis set with RB3LYP functions was employed in all calculations. This method has been proven to produce more reliable geometries and vibrational frequencies for 1-vinyl-3-alkylimidazolium salt systems.

2.3. Viscosity and conductivity measurements

The conductivities and viscosities of the five pure ionic liquids were examined by a DDSJ-308A conductivity meter (Shanghai Precision & Scientific Instrument Co., Ltd.) and an NDJ-79 rotational viscosimeter (Shanghai Ande Instrument Equipment Co., Ltd.) at room temperature in air, respectively.

2.4. DSSC fabrication

TiO₂ nanoparticle powder (6.0 g, Degussa P25), glacial acetic acid (12 g), ethyl cellulose (2.0 g), polyethylene glycol (2.0 g, F.W. 20,000), and Triton X-100 (0.1 mL) were added into a mortar and ground to form a slurry. Through screen-printing technique the slurry was spread onto SnO₂:F conducting glass (FTO, fluorine-doped SnO₂, sheet resistance 10 Ω/cm², Asahi) and allowed to dry on the surface of the barrier layer at 80 °C overnight in vacuum oven. After the substrate was sintered at 450 °C for 30 min and cooled down to 80 °C, the TiO₂ thin film electrode was immersed in a 0.3 mM N3 (N3, Dyesol) dye/ethanol solution overnight. The composition of the electrolyte was 0.6 M 1-vinyl-3-alkylimidazolium iodide, 0.06 M iodine, 0.5 M 4-tertbutylpyridine (TBP) and different contents of lithium iodide (0, 0.2, 0.4 and 0.6 M) in propylene carbonate. A sandwich-type configuration with active area 0.20 cm² consisted of N3-sensitized TiO₂ thin film electrode, a Pt-coated FTO counter electrode and ionic liquid electrolytes. Photocurrent–photovoltage characteristics of solar cells were measured by a Keithley model 2400 digital source meter using an Oriel 91192 solar simulator equipped with AM 1.5 filter and intensity 100 mW/cm².

2.5. Photovoltaic characteristics

Fig. 2 offers a sketch of main photovoltaic parameters such as *J*_{sc}, *V*_{oc}, fill factor (FF) and *η*. The short-circuit photocurrent density (*J*_{sc}) equals the current intensity of the unit area when the applied bias potential is zero. The open-circuit photovoltage (*V*_{oc}) is the cell potential when the photocurrent is zero, corresponding to almost flat valence and conduction bands. FF is obtained by a full current–voltage characterization. This quantity is essentially a measure of the diode behavior of the cell. The efficiency (*η*) describes the overall photon-to-current conversion of the cell. The formulae of these two important parameters are as follows:

$$FF = \frac{V_{\max} J_{\max}}{V_{oc} J_{sc}} \quad (1)$$

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