

Influence of tagging thiophene bridge unit on optical and electrochemical properties of coumarin based dyes for DSSCs with theoretical insight

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ABSTRACT

A novel series of coumarin based dyes were designed and synthesised with coumarin donor (D) moiety, various thiophene bridge (Th- π) unit and –CNCHCOOH acceptor (A). The dye sensitized solar cells' (DSSCs) performance, optical and electrochemical properties of coumarin dyes were examined systematically. Moreover, optimization calculations for the geometries of all the coumarin dyes with various Th-bridge units were studied by DFT (density functional theory). CDT-3 dye containing three Th- unit shows the highest short circuit current (J_{sc} = 15.14 mA/cm²) and efficiency is 6.02% under 1 sunlight (100 mW/cm², AM1.5) illumination. The DSSCs devices with all three coumarin dyes exhibit good, long term stability up to 500hr.

1. Introduction

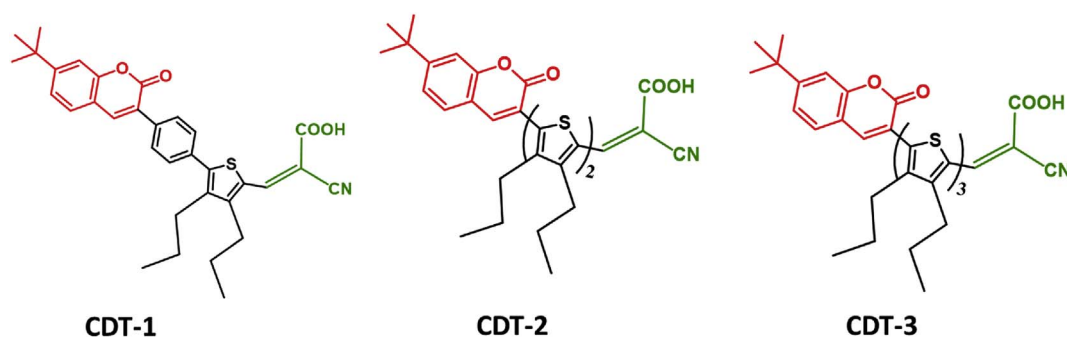
The solar light is converted into electricity by dye sensitized solar cells (DSSCs) and this phenomenon has been broadly studied since the work of M. Gratzel research group [1]. DSSCs has concerned sustainable attention due to their so many advantages such as easy fabrication process, low materials cost, high power conversion efficiency (η) and subtract flexibility [2–4]. DSSCs with using ruthenium based dye (N719, N3) showed noticeable results up to 12% efficiency [3]. These ruthenium dyes having some drawbacks like its toxicity, cost-factors etc, and some modifications are required. To avoid this problem organic metal free dyes, which are cheaper, controllable absorbance maxima, flexibility in design and synthesis process, are widely used these days [5,6]. The higher photo conversation efficiency reported by metal free dyes have driven further analysis. As per literature, many types of donor (D) and bridge (π) moieties used such as carbazole [7], triphenylamine [8], coumarin [9], phenothiazine [10], thiophene [11], benzene [12], furan [13], etc. Among them coumarin donor moiety is widely used as commercially significant florescent materials due to their sufficient fluorescence in the visible region and good quantum yield of photoluminescence. The organic metal free dyes employed for DSSCs so far, coumarin dyes are one kind of capable dye stuff [14] and have been studied systematically in our

previous work [5]. Hara and co-workers first time used coumarin dye having conjugated system using a methane moiety, which has given 5.60% efficiency for photovoltaic device [15]. The substitution of bulky moieties that prevent aggregation enhanced the efficiency up to 6.6% [16]. In 2007, Wang et al. reported Th- substituted coumarin dye with co-adsorption of deoxycholic acid (CDA) to achieved 7.6% efficiency [17]. In 2008, the same research group has increased Th-moiety in bridge position to studied influence on efficiency and other photovoltaic parameters [18]. By prolonging the π -bridge by a Th- π moiety, which could be enhanced the efficiency to 7.65% [19].

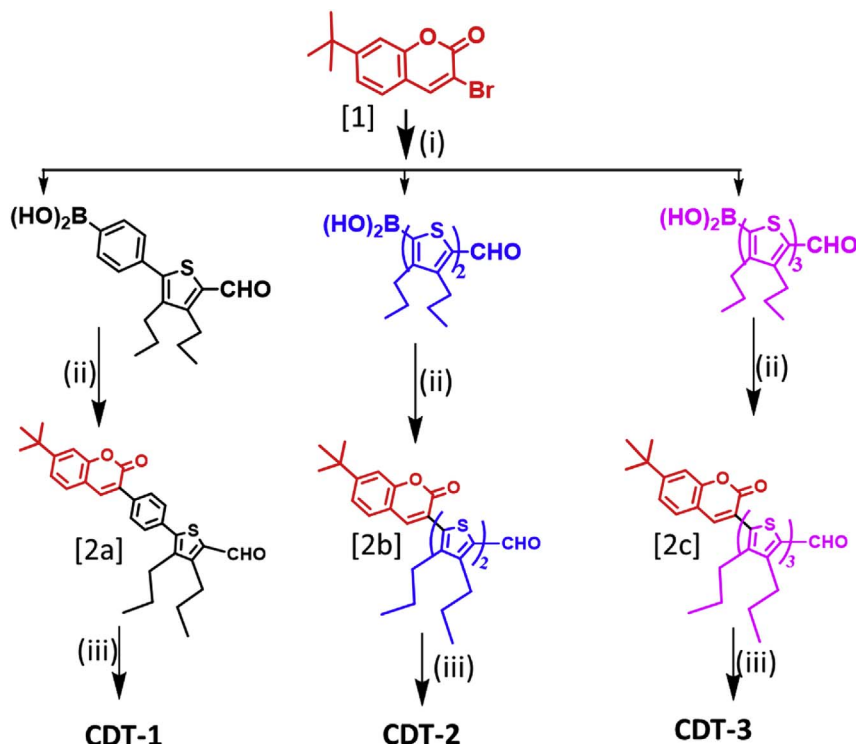
Later on, substituting a Th- moiety based π -bridge in between the donor (D) and anchoring (A) group to the push–pull structure, the stability under 1 sun illumination and the efficiency were further improved, reaching near to 8.2% efficiency. In 2012, Kim and co-workers have been reported D-A- π -A coumarin donor moiety based dye having benzothiadiazole with efficiency 5.9% [20]. Yu and co-workers designed coumarin dye based on a two D- π -A dyes to reduced aggregation and increasing the efficiency [21]. While coumarin dyes based DSSCs were little known regarding the relationship between the structural geometry and efficiency.

These studies point out the further chemical modifications of these coumarin moiety based dyes may produce higher efficiency. On the

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Scheme 1. Chemical structure of coumarin dyes.

Scheme 2. Synthesis routes of the coumarin dyes. (i) coumarin amine derivative, CCl_3 , NBS, 75 °C, (ii) boronic acid derivatives, KCO_3 , $\text{Pd}(\text{PPh}_3)_4$, DMF, toluene, 95 °C at 24hr stirring, (iii) $-\text{CNCHCOOH}$, pipyridine, CCl_3 .

basis of D- π -A structure concept, we have synthesised a series of coumarin based chromophore dyes by substituting various number of Th moiety unit as bridge to connect D and A (Scheme 1). The minor change in dye bridge unit will result in different and interesting electrochemical, optical and photovoltaic performance. By increasing the Th-bridge unit in coumarin dye, results in increasing the short circuit current (J_{sc}) and overall efficiency (η). Three thiophene unit based CDT-3 dye generated highest efficiency 6.02% ($J_{sc} = 15.04 \text{ mA/cm}^2$, $V_{oc} = 0.722 \text{ V}$, FF = 0.56) compared to CDT-1 and CDT-2. The optimization of all coumarin dyes geometry-calculations was done by density function theory (DFT) using B3LYP/6-31G (d,p) basis set. A long term stability of synthesised coumarin dye showed up to 500hr in presence of 1 sun illumination (100 mW/cm^2 , AM 1.5).

2. Experimental section

2.1. Materials and methods

All the reactions were carried out under a nitrogen atmosphere. The preparation of starting materials were synthesised according to previous literature [5]. The (4-(5-formyl-3,4-dipropylthiophen-2-yl)phenyl)boronic acid, (5'-formyl-3,3',4,4'-tetrapropyl-[2,2'-bithiophen]-5-yl)boronic acid, (5''-formyl-3,3',3'',4,4',4''-hexapropyl-[2,2':5,2'':

terthiophen]-5-yl)boronic acid, coumarin were purchased from Sigma-Aldrich. The ethyl cellulose, alpha-terpineol, TiO_2 nanocrystalline were purchased from Sigma-Aldrich and used as received. The solvents were distilled freshly according to standard procedures. Meltonix tap ($25 \mu\text{m}$) and fluorine doped tin oxide (FTO) glass ($12 \Omega/\text{cm}^2$) were procured from Solaronix Switzerland.

2.2. Photovoltaic device assemble

The conducting FTO glass was washed with surfactant, water and alcohol solvent using ultrasonic bath for 10 min. The preparation of photoanode was done following our previous paper procedures [5,22,23], in short, the TiO_2 paste was deposited by doctor blading and calcinate up to 450 °C for 30min. After being cooled to 60 °C, the TiO_2 photoelectrode (thickness $\sim 12 \mu\text{m}$) was added into the coumarin dye (30 mmol) solution in a mixture of ethanol and chloroform and kept at overnight to assure complete dye sensitized. The Pt-counter electrodes were prepared by spine coated Pt salt solution on FTO substrate at 1500 rpm and calcined 450 °C at 10min in furnace. Open cells were assembled in air by clamping the different photo electrodes with counter electrodes. The electrolyte I-/I₃⁻, which contains 0.5 M 3-butyl-N-methyl imidazolium iodide (BIMI), 50 mM TBP, 50 mM I₂ in 3-methoxy propionitrile. The DSSC devices active area was 0.25 cm².

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