

Achieving Efficient Solution-Processed Small Molecular Solar Cells via Non-halogenated Solvent

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Abstract

Non-halogenated solvent has been used to fabricate efficient solution-processed small molecule solar cells. Power conversion efficiency (PCE) of 5.6% has been achieved using toluene compared to 4.8 % using chloroform (CF). These are promising results towards replacing the toxic halogenated solvents commonly used in organic photovoltaics (OPVs) with more eco-friendly solvents.

1. Introduction

Toxic halogenated solvents such as chloroform (CF) are commonly used in OPVs devices fabrication mainly because of their good solubility performances. That is the reason why most of the highest efficiencies in OPVs have been achieved using halogenated solvents (i.e. CF) reaching 10% [1]. From industry point of view, toxic solvents are being considered a big obstacle facing OPVs upscaling and large area production. Therefore, there is an urgent need to find alternative solvents to replace the halogenated toxic ones [2]. These alternatives should maintain similar or even higher performances relative to halogenated solvents beside their eco-friendly nature. Many attempts have been reported in the last few years to find eco-friendly solvents capable of competing halogenated counterparts.

Non-halogenated solvents have been applied in both solution-processed polymer and molecular solar cells. In the former, the highest reported PCE is 9.5% achieved using *o*-xylene with 1% of anisaldehyde as solvent additive [3]. However, in solution-processed molecular solar cells, few reports have been published using non-halogenated solvents. Bazan et al. [4] achieved maximum PCE of 5% using *o*-xylene with 1% of anisaldehyde as solvent additive [3]. However, in solution-processed molecular solar cells, few reports have been published using non-halogenated solvents. Brabec et al. introduced blend system composed of N(Ph-2T-DCN-Et)₃ as a small molecule donor with PC₇₁BM as acceptor dissolved in solvent mixture of benzaldehyde:mesitylene with ratio of (80:20) as non-halogenated solvent. They reached PCE of 3.7% which is comparable to results obtained using chlorobenzene [5].

Here we report solution-processed molecular OPVs fabricated from toluene as non-halogenated solvent. Two-dimensional conjugated small molecule (SMPV1) [6]

with [6,6]-phenyl-C₇₁-butyric acid methyl ester (PC₇₁BM) composed bulk heterojunction (BHJ) active layers casted from toluene. Compared to devices fabricated from CF, the as-cast devices composed of SMPV1:PC₇₁BM processed from toluene achieved PCE of 5.6% without any further treatment. While that fabricated from CF under the same conditions achieved PCE of 4.8%. From these results we can conclude that toluene is a good candidate to replace CF in this molecular blend system.

2. General Instructions

Fig. 1 shows organic materials and solvents used in this work. SMPV1 (purity: >99%) was obtained from Luminescence Technology (Lumtec). PC₇₁BM was purchased from Solenne b.v. Toluene and chloroform solvents were purchased from Sigma Aldrich.

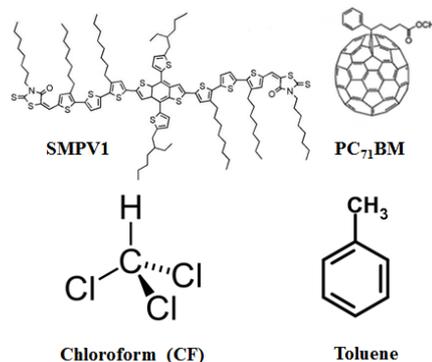


Fig. 1 Chemical structures of organic materials and solvents used in this work.

Conventional device structure of (ITO/PEDOT:PSS/SMPV1:PC₇₁BM/Ca/Al) has been used. SMPV1:PC₇₁BM blend system with ratio of 1:0.75 and donor concentration of 15 mg/ml has been used to form active layers casted from toluene. While for CF blend ratio of 1:0.8 and 8 mg/ml donor concentration have been used. Ca/Al electrode was deposited through thermal evaporation in a vacuum chamber.

Photovoltaic characteristic current-voltage curves (*J-V*) for devices processed from toluene and CF are shown in Fig. 2 (a). Devices fabricated from toluene achieved short circuit current (*J_{sc}*) of 10.33 mA cm⁻², voltage (*V_{oc}*) of 0.95 V and fill factor (FF) of 56% leading to PCE of 5.6%. While devices processed from CF achieved PCE of 4.8%

with device parameters of ($J_{sc}=9.80 \text{ mA cm}^{-2}$, $V_{oc}=0.91 \text{ V}$ and $FF=54.16\%$). External quantum efficiency (EQE) of these devices is shown in Fig. 2 (b). Devices processed from both toluene and CF showed the same EQE behavior covering the entire absorption range from 300 to 700 nm. Consistent with $J-V$ curves, EQE peaks at 550 nm for devices processed from both toluene and CF are 56% and 52% respectively. Aiming to replace the halogenated, toxic solvents used in molecular OPVs fabrication with less toxic and eco-friendly solvents such as toluene, results reported here are promising. We believe that with further optimization, we can push the PCE more reaching close to 7%.

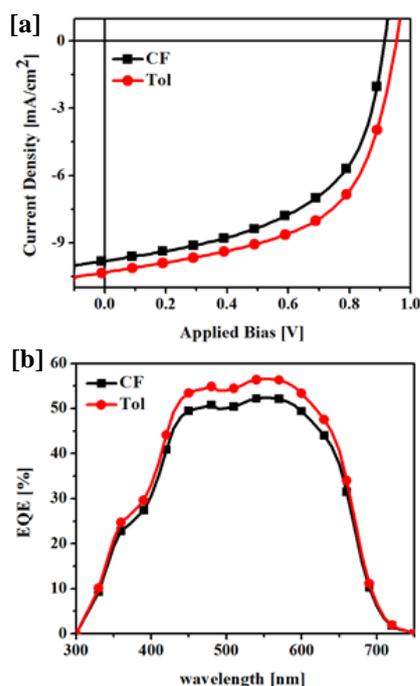


Fig. 2 (a) $J-V$ photovoltaic characteristic curves for devices fabricated from toluene and CF (b) their corresponding EQE.

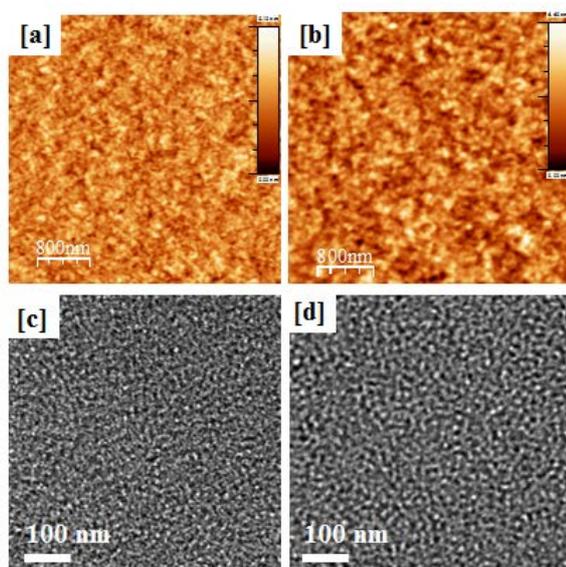


Fig. 3 (a) and (c) show AFM and TEM images for active layers casted from CF while (b) and (d) show AFM and TEM images for

active layers casted from toluene.

Fig. 3 shows a comparison between morphology of the active layers processed from CF as halogenated solvent and toluene as non-halogenated solvent. Atomic force microscopy (AFM) and transmission electron microscopy (TEM) have been used to investigate the active layers morphologies. Fig. 3 (a) and (b) show AFM images of active layers processed from CF and toluene respectively. Both films showed slight differences in morphologies with similar roughness of 0.86 nm. This means that toluene as non-halogenated solvent has the ability to achieve the favorable phase separation required for charge transfer. Corresponding TEM of active layers processed from CF and toluene are shown in Fig. 3(c) and (d) respectively showed good agreement with AFM images. Similarities in morphologies obtained from CF and toluene demonstrate similar ability of the two solvents to organize the BHJ components within the timescale of film formation.

3. Conclusions

In conclusion, we present efficient molecular OPV processed from toluene as non-halogenated solvent. SMPV1:PC₇₁BM blend system processed from toluene achieved PCE of 5.6% which is higher than that obtained using CF (4.8%). These results are a step on the way towards upscaling and OPVs industrialization. Our results are among the highest reported PCE in molecular OPVs casted from non-halogenated solvents. Further optimizations and characterizations are ongoing for insight understanding of non-halogenated solvents in molecular OPVs in order to reach higher performances.

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