A step in investigating commercial viability of high performing OPV materials on a cost/kWh basis

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The field of polymer solar cells has experienced rapid growth during the last decade. This has led to an astonishing record power conversion efficiency (PCE) just short of 20%. However, the challenge of commercialisation, except for niche applications, remain. Further efforts are needed to address the discrepancy in power conversion efficiency between laboratory scale devices and large scale devices as well as to address the lack of research on upscaling and development of high-performance materials with low synthetic complexities.

The 10-10 target (PCE of 10%, lifetime of 10 years) has often been considered the limit for commercial viability. However, this is not necessarily correct, instead the only measure that is relevant for commercialisation is the total cost per kWh produced. Simplified, the total cost per kWh is dependent on material costs, manufacturing costs, installation costs, lifetime, and PCE. In order to elucidate the cost contribution of the active layer, the synthesis costs of promising donors and acceptors should be investigated.

In this study, the cost of the popular acceptor ITIC as well as the cost of two high performing donor polymers, namely PBDB-T and PDCBT, were investigated. The synthesis cost of these 3 materials were calculated according to published literature procedures, using estimations from Osedach et. al.[1] where weights and volumes could otherwise not be obtained. Quotes to determine pricing for reactants, reagents and solvents were restricted to laboratory quantities (i.e., no bulk pricing) and larger companies were chosen over smaller suppliers if possible. Furthermore, power costs, consumables used for cleaning as well as items such as syringes and filter papers were excluded from the cost calculations. To easier track the origin of high-cost items/procedures the calculated costs were divided into reaction costs and purification costs.

In the case of ITIC the synthesis costs were determined for two different scenarios. In scenario 1 the costs were calculated following the literature procedures, as described above. In scenario 2 these assumptions were tested experimentally and ITIC was synthesised on a ≥10 g scale. In this second scenario the literature procedures were modified with an aim of lowering overall synthesis costs. However, post optimisation the experimental synthesis route only deviated slightly from the literature procedures.[2-4] In the 5-step synthesis procedure the largest differences were found in the purification procedures. The reaction procedures in synthesis steps 1-3 remained almost identical for the formation of the core IT-CHO unit even after optimisation. On the purification side the removal of a chromatography process in synthesis step 3 and a recrystallisation in synthesis step 4 contributed to a lower cost profile. Minor changes in reaction step 4 also contributed to a lower cost, but the largest overall contributor was the increase in the yield of step 5, where the side groups are linked to the IT-CHO core forming the final product, from 21% to 73%. The calculations revealed a high cost of $257/g for ITIC for scenario 1. In scenario 2 the cost was calculated to $52/g, this is equivalent to 1/5 of the cost of scenario 1 (or about 4% of the cost of commercially available ITIC). This provides an indication that all synthesis costs need to be experimentally confirmed at scale.

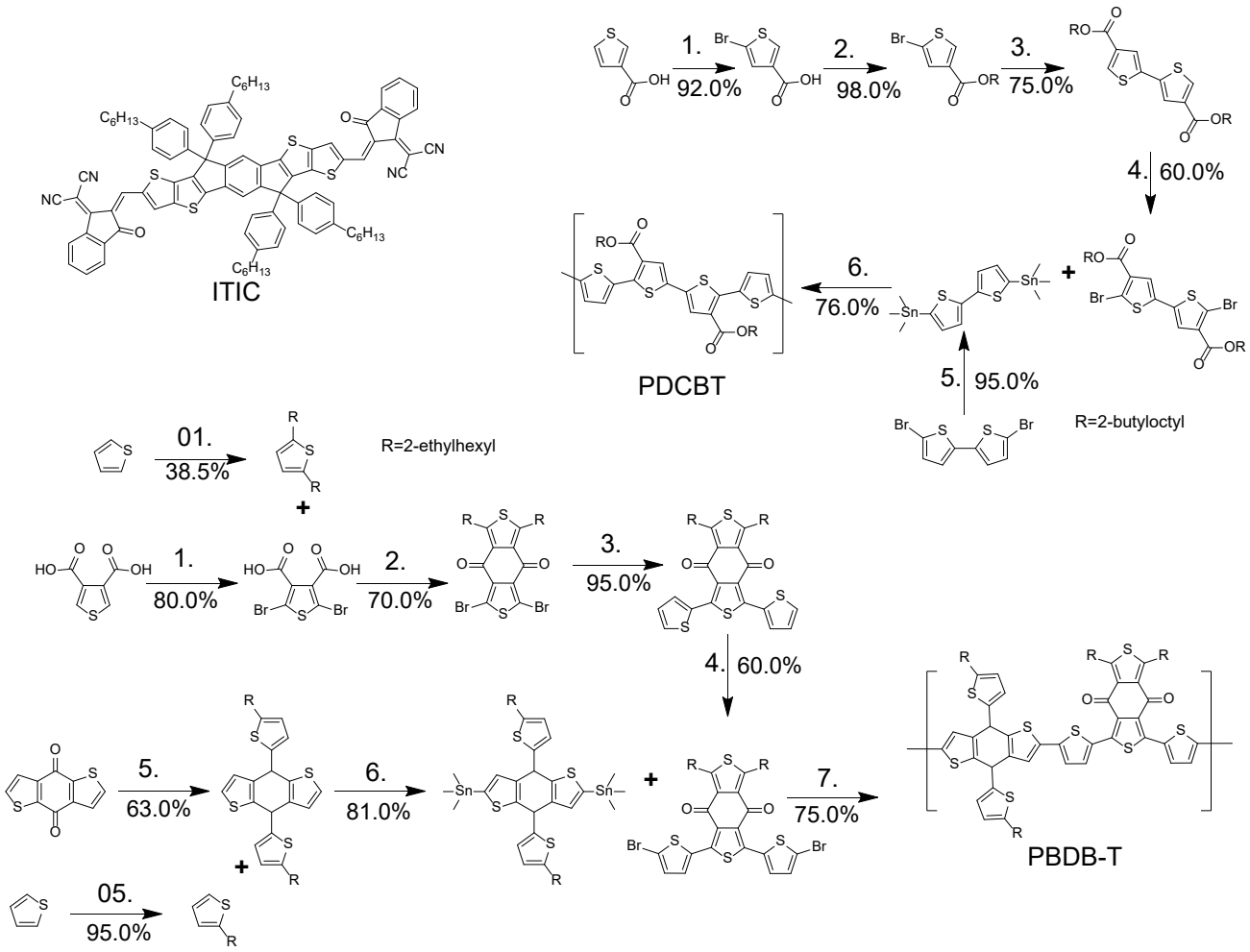

Figure 1. Molecular structure of ITIC and synthesis schemes for PBDB-T and PDCBT

Following the same procedure as in scenario 1 for ITIC, synthesis costs were also calculated for donor polymers PBDB-T[5-10] and PDCBT[11-12]. The 8-step synthesis route of PBDB-T and the shorter 6-step synthesis route of PDCBT is presented in Figure 1. More steps tend to correlate to an increased synthetic complexity which in turn indicates a higher cost. This is also the case here; the calculation reveals a cost of $103/g for PBDB-T and $54/g for PDCBT. Assuming an active layer thickness of 150 nm, a D:A ratio of 1:1, a 50% reduction in PCE[13-14] from laboratory scale to large scale, a 1-year lifetime, and a 50% geometric fill factor, the cost contribution of the two active layer materials synthesis to the cost per kWh was calculated. These assumptions yielded a cost of $0.1255/kWh for PBDB-T:ITIC and $0.0951/kWh for PDCBT:ITIC. When comparing these costs in $/MWh to the LCOE of established technologies, see Table 1, it is clear that the active layer costs alone are quite high. Nevertheless, improvements in the cost profile can be expected as economy of scale will reduce active layer materials costs if/when the technology is moving toward commercialisation. It is also important to note that the lifetime will have a big impact on the cost/kWh and that a short lifetime purposefully was assumed in this study.

Table 1. Active layer costs compared to LCOE for established technologies.

LCOE for Active Layers vs Established Technologies [$/MWh]				
PBDB-T:ITIC	PDCBT:ITIC	Solar	Wind	Gas
125.5	95.1	47	58	81

There are numerous publications detailing synthesis on the mg scale or device fabrication of high performing active layers on small glass substrates. On the other hand, only a small number of studies are investigating materials and deposition processes with respect to large scale viability. In this study, one way of investigating the cost contribution of the active layer to the final device was detailed. High active layer costs were determined for both PBDB-T:ITIC and PDCBT:ITIC donor:acceptor pairs, showing the importance of setting a precedent on how to approach commercial viability. Further, the study highlights the importance of economies of scale for commercial production, and that favourable economics shouldn't be perceived as the inevitable outcome of upscaling. As a last point, the lack of studies taking a purely economic standpoint could on a longer timeframe delay a potential market entry of a low carbon technology.

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