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Effect of synthetic accessibility on the commercial viability of organic photovoltaics†

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For organic photovoltaics (OPVs) to become a viable source of renewable energy, the synthesis of organic active-layer materials will need to be scaled to thousands of kilograms. Additionally, the ultimate cost of these materials will need to be low enough to constitute only a small fraction of the cost of the solar cell module. In this study, we present a quantitative analysis, based on published small-scale synthetic procedures, to estimate the materials costs for several promising OPV materials when produced in large quantities. The cost in dollars-per-gram ($ per g) is found to increase linearly with the number of synthetic steps required to produce each organic photoactive compound. We estimate the cost-per-Watt ($ per W_p) as a function of power conversion efficiency (PCE) for an archetypal OPV structure and find that a relatively simple molecule requiring only 3 synthetic steps will contribute a cost of 0.001 to 0.01 $ per W_p, given a solar module PCE of 10%. In contrast, a relatively complicated molecule requiring 14 synthetic steps will contribute costs in the range of 0.075 to 0.48 $ per W_p. Our findings suggest that the commercial viability of an OPV technology may depend on the synthetic accessibility of its constituent active layer materials. Additionally, this work stresses the importance of optimizing synthetic routes to minimize solvent and reagent usage as well as to minimize the number of required workup procedures in the scaled production of OPV materials.

Broader context

For organic photovoltaics (OPVs) to become a viable source of renewable energy, the synthesis of organic active-layer materials will need to be scaled to thousands of kilograms. Additionally, the ultimate cost of these materials will need to be low enough to constitute only a small fraction of the cost of the solar cell module. In this study, we present a quantitative analysis, based on published small-scale synthetic procedures, to estimate the materials costs for several promising OPV materials. The cost in dollars-per-gram ($ per g) is found to increase linearly with the number of synthetic steps required to produce each organic photoactive compound. We estimate the cost-per-Watt ($ per Wp) as a function of power conversion efficiency (PCE) for an archetypal OPV structure and find that relatively complicated molecules (>6 synthetic steps) may represent a considerable fraction of the cost of an organic solar cell. Our findings suggest that the commercial viability of an OPV technology may depend on the synthetic accessibility of its constituent active layer materials. Additionally, this work stresses the importance of optimizing synthetic routes to minimize solvent and reagent usage as well as to minimize the number of required workup procedures in the scaled production of OPV materials.

Introduction

The development of organic photovoltaics (OPV) is widely considered to be a viable route for the realization of low-cost renewable energy.[1] There are several factors that justify this optimism. The inherent low cost of many organic semiconductors including small molecules and conjugated polymers, combined with the compatibility of these materials with low-temperature processing techniques, suggests the possibility to realize a new generation of inexpensive PV modules. The considerable progress in improving the performance of OPV structures over the past decade (see Table 1), has led to a recent report on a polymer-based tandem solar cell structure, for example, which has demonstrated a power conversion efficiency (PCE) exceeding 8%.[2] It is expected that the engineering of new organic materials and device structures may yield even greater photovoltaic performance in the coming decades.[3]

Considerable attention is now focused on developing specialized organic semiconductors that are engineered to serve as active layer materials in OPV structures.[4] These efforts aim to enable

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† Electronic supplementary information (ESI) available: Schemes and flowcharts describing the synthesis of **Alq3**, **DBP**, **SQ**, **DTS**, **PDPP3T** and **PBDTTPD**. Additional discussion of isolation and purification. Raw material prices. Plots of C_W *versus* efficiency for additional materials. See DOI: 10.1039/c3ee24138f

Table 1 Survey of recent OPV structures. Donor and acceptor materials, as well as the maximum PCE under AM1.5 illumination, are indicated

Year	Donors[b]	Acceptors[b]	PCE [%]
2011 (ref. 2)	**P3HT**, PBDTT-DPP	ICBA, PC$_{71}$BM	8.62[a]
2009 (ref. 7)	PBDTT-CF	PC$_{71}$BM	6.77[a]
2012 (ref. 8)	**DTS**	PC$_{71}$BM	6.70
2009 (ref. 9)	PCDTBT	PC$_{71}$BM	6.10[a]
2010 (ref. 10)	**PBDTTPD**	PC$_{71}$BM	5.50
2009 (ref. 11)	**PTB1**	PC$_{61}$BM, PC$_{71}$BM	5.30
2009 (ref. 12)	BP(CP)	SIMEF	5.20
2008 (ref. 13)	**P3HT**, PBDTT-DPP	PC$_{61}$BM	5.16
2010 (ref. 14)	**SQ**	C$_{60}$	4.60
2007 (ref. 15)	**CuPc**	C$_{60}$	4.40
2009 (ref. 16)	**PDPP3T**	PC$_{61}$BM	3.80
2009 (ref. 17)	**DBP**	C$_{60}$	3.60
2010 (ref. 18)	ClAlPc	C$_{60}$	3.00
2009 (ref. 19)	ClAlPc	C$_{60}$	2.00

[a] Chemical abbreviations: **P3HT** = poly(3-hexylthiophene); PBDTT-DPP = poly[2,6′-4,8-di(5-ethylhexylthienyl)benzo[1,2-*b*;3,4-*b*]dithiophene-*alt*-5-dibutyloctyl-3,6-bis(5-bromothiophen-2-yl)pyrrolo[3,4-*c*]pyrrole-1,4-dione]; PBDTT-CF = poly[4,8-bis(2-ethylhexyloxy)-benzo[1,2-*b*:4,5-*b*′]dithiophene-2,6-diyl-*alt*-(4-octanoyl-5-fluoro-thieno[3,4-*b*]thiophene-2-carboxylate)-2,6-diyl]; **DTS** = 5,5-bis(4-(7-hexylthiophen-2-yl)thiophen-2-yl)-[1,2,5]thiadiazolo[3,4-*c*]pyridine-3,3-di-2-ethylhexylsilylene-2,2′-bithiophene; PCDTBT = poly[2,1,3-benzothiadiazole-4,7-diyl[4,4-bis(2-ethylhexyl)-4*H*-cyclopenta[2,1-*b*:3,4-*b*′]dithiophene-2,6-diyl]; **PBDTTPD** = poly((4,8-diethylhexyloxyl)benzo([1,2-*b*:4,5-*b*′]dithiophene)-2,6-diyl)-*alt*-((5-octylthieno[3,4-*c*]pyrrole-4,6-dione)-1,3-diyl); **PTB1** = poly((4,8-bis(octyloxy)benzo(1,2-*b*:4,5-*b*′)dithiophene-2,6-diyl)(2-((dodecyloxy)-carbonyl)thieno(3,4-*b*)thiophenediyl)); BP = tetrabenzoporphyrin; CP = 1,4:8,11:15,18:22,25-tetraethano-29*H*,31*H*-tetrabenzo[*b*,*g*,*l*,*q*]porphyrin; SIMEF = 1,4-bis(dimethyl-phenylsilylmethyl)[60]fullerene; **SQ** = 2,4-bis[4-(*N*,*N*-diisobutylamino)-2,6-dihydroxyphenyl]squaraine; **CuPc** = copper phthalocyanine; **PDPP3T** = poly[(2,5-bis(2-hexyldecyl)-2,3,5,6-tetrahydro-3,6-dioxopyrrolo[3,4-*c*]pyrrole-1,4-diyl)-*alt*-([2,2′:5′,2′-terthiophene]-5,5′-diyl)]; **DBP** = dibenzo([*f*,*f*′]-4,4′,7,7′-tetraphenyl)diindeno[1,2,3-*cd*:1′,2′,3′-*lm*]perylene; ClAlPc = chloro-aluminum phthalocyanine; ICBA = indene C$_{60}$ bisadduct; PC$_{71}$BM = phenyl C$_{71}$ butyric acid methyl ester; PC$_{61}$BM = phenyl C$_{61}$ butyric acid methyl ester. [b] Certified by NREL.

high performance by realizing materials that simultaneously exhibit high optical absorption coefficients, high carrier mobilities and carefully engineered energy band alignments suitable for exciton dissociation. Presently, much of this work is conducted at a relatively small scale, conducive to laboratory experiments. However, a successful and broadly deployable OPV technology will require the chemical synthesis of the constituent active materials to be scaled from the level of grams-of-product to thousands-of-kilograms, sufficient for the widespread deployment of OPVs.‡ Simultaneously, these large-scale synthetic processes must achieve low enough material costs to represent only a small contribution to the cost of the solar cell module. This scalability challenge is the focus of the analysis of the present study. In particular, we focus on donor materials, which are generally the most structurally complex organic constituents of OPV structures.

Some insight into the large-scale production of photoactive OPV materials may be gained by consideration of pharmaceutical drugs. Pharmaceutical drugs, which are often complex molecular compounds that require multi-step syntheses, are similarly subject to imperatives for large-scale and low-cost manufacturing processes. In the pharmaceutical industry, the "synthetic accessibility" of prospective target molecules is of paramount concern as it strongly affects the cost and environmental impact of the manufacturing process required to synthesize appropriate quantities of a particular drug.[5] Synthetic accessibility refers to the various factors that determine the ease with which a particular molecule can be synthesized. These include the commercial availability and/or accessibility of reagents, the number and difficulty of synthetic steps, the stability of intermediate products, the potential for combining steps together ("telescoping"), and yield.[6] Although achieving high synthetic accessibility is recognized to be critical to the pharmaceutical industry, very little consideration has so far been given to the importance of this quality with regard to prospective materials for organic solar cells. For a broad deployment of OPV technologies, the photoactive materials would need to be synthesized at an even larger scale than pharmaceutical drugs to meet global energy needs.

In this work, we investigate the relationship between synthetic accessibility and material cost for several OPV materials. One of the challenges associated with addressing this topic is that very little data on specific synthetic routes is publicly available for large-scale procedures used in industry. This is due in part to a lack of relevant case studies of scaled OPV materials and also to the sensitive and competitive nature of such proprietary details. Here, we address this problem by basing our study on small-scale procedures that are available in published literature. We present a detailed quantitative analysis that takes into account all of the material inputs to these procedures in order to estimate the total material costs for several photoactive materials. We then assume an archetypal OPV structure to consider how these material costs would affect the commercial viability of OPV structures as a function of solar cell efficiency.

Methods

Materials of interest

We consider nine organic materials of interest (see Fig. 1) that span a wide range of complexity and synthetic accessibility. These include the small molecules **CuPc**,[15,20] **SQ**,[14,21] **DBP**[17] and **DTS**,[8] as well as the polymers **P3HT**,[13] **PDPP3T**,[16] **PTB1**[11] and **PBDTTPD**.[10] Each of these materials has been used in OPV demonstrations, as summarized in Table 1. Although not explicitly of interest for organic solar cells, we also include the small molecule, **Alq3**, which is an archetypical electron-transporting material in organic light emitting diodes (OLEDs)[22] and has been a benchmark organic optoelectronics material since the 1980's.

A relatively inexpensive OPV material is copper phthalocyanine (**CuPc**), which is a broadly used electron donor material for organic solar cells.[15,20,23] The synthesis of **CuPc** consists of a

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‡ We assume a solar cell with a PCE of 10% and in which the organic active layer has a thickness of 100 nm and density of 1.1 g cm^{-3}. To generate 1 GW of electricity under peak illumination conditions, 1100 kg of organic material will be required (not accounting for material that is wasted during deposition).

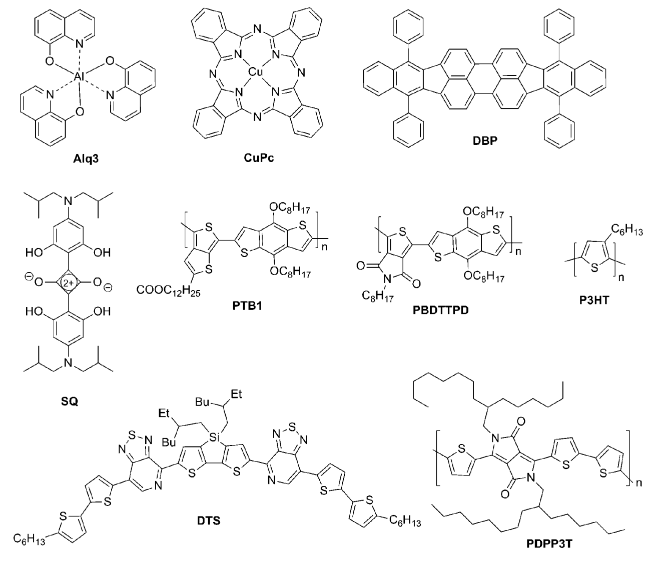


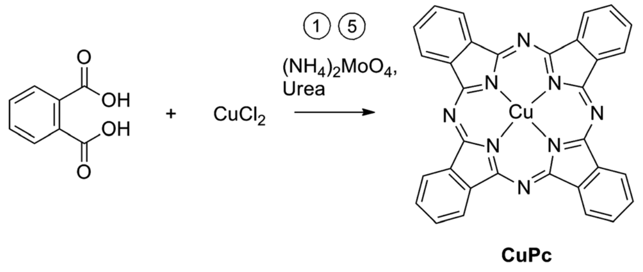
Fig. 1 Organic molecules considered in this study.

single step.[24] Due to its widespread use as a colorant and pigment, **CuPc** is already manufactured at a scale of millions of kg-per-year, and is available for less than 1 dollar-per-gram.[25] In contrast, many of the most promising OPV active layer materials involve highly specialized and complex synthetic procedures and are consequently available only in small quantities and at a relatively high cost. A representative example is the polymeric material **PTB1**, which was used as an electron donor to realize an OPV structure with a PCE of 5.3%.[11] Due to its highly specialized nature and relatively complicated synthesis, which consists of 14 individual steps,[26–29] this molecule is presently available only from a single supplier at a cost of several thousand dollars-per-gram.

Synthetic accessibility

There are several factors that affect the synthetic accessibility of a molecule. Among these are a variety of chemical as well as logistical considerations. The lack of a rigorous definition for this quality makes its determination and comparison among different molecules a non-trivial task.[5] For simplicity, we use the number of synthetic steps (here delineated by the number of explicit isolations required during synthesis) needed to produce the material as a metric for its synthetic accessibility; the greater the number of steps, the less "accessible" the molecule is to industry.[6] This choice enables us to compare and quantify the complexity of different molecules in a very simple and intuitive manner. One qualification, however, pertains to the choice of starting material for each of the synthetic procedures. For the procedures considered in this study, we regard the beginning of the procedure to be the point at which the starting materials are simple molecules that are currently available from bulk chemical suppliers. However, recognizing the shifting nature of small chemical enterprises, we estimate a ±2 step error in our analysis.

We identified detailed literature procedures for the synthesis of each of the molecules shown in Fig. 1. In each case, we chose synthetic routes with the highest overall yields if multiple reported synthetic methods were available. The procedures for **CuPc**, **P3HT** and **PTB1**, representing a range of complexity, are shown in Schemes 1–3. Schemes describing the synthesis of the remaining molecules (**SQ**, **DBP**, **Alq3**, **DTS**, **PDPP3T** and **PBDTTPD**) are available in the ESI.† The number of synthetic steps for each molecule was extracted from these schemes.



Scheme 1 Synthesis procedure for **CuPc**. Circled numbers represent specific workup procedures, as described in the text.

Isolation and purification

An important aspect of synthetic procedures is the isolation (often termed "work-up") and purification of desired products from a crude reaction mixture (see ESI for additional discussion†). With regard to our analysis, consideration of workup and purification operations adds considerably to the material inputs and waste outputs for each procedure. To ensure a fair comparison among different synthetic routes, we created a framework with which to evaluate the material requirements for these workup and purification steps. We include operations for (1) quenching/neutralization, (2) extraction, (3) column chromatography, (4) recrystallization and (5) distillation/sublimation. The details for each type of workup procedure are based on standard organic laboratory techniques[30] and are elaborated individually below.

1 **Quenching/neutralization.** These procedures were evaluated on a case-by-case basis. One-to-one molar equivalents of acid, base, or water were assumed to be necessary to neutralize reactive reaction intermediates or side-products, as necessary.

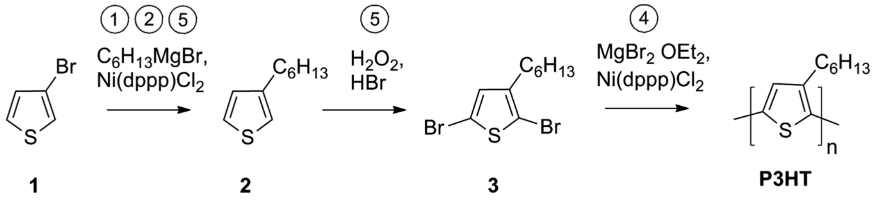
2 **Extraction.** The use of 150 mL solvent (three individual 50 mL extractions) and 1 g of a drying agent (Na_2SO_4, or $MgSO_4$) is assumed to be necessary to extract 1 g of crude product from a reaction mixture. These numbers are proposed as an upper limit to the total solvent and material use necessary to isolate the product of a reaction.

3 **Column chromatography.** An ideal separation ratio ($R_f > 0.3$) and sample loading is assumed.[31] We assume 2.5 g sample and 1 L of effluent are used in a column that is 20 cm long 50 mm in diameter. We assume that 60 μm SiO_2 particles are used.

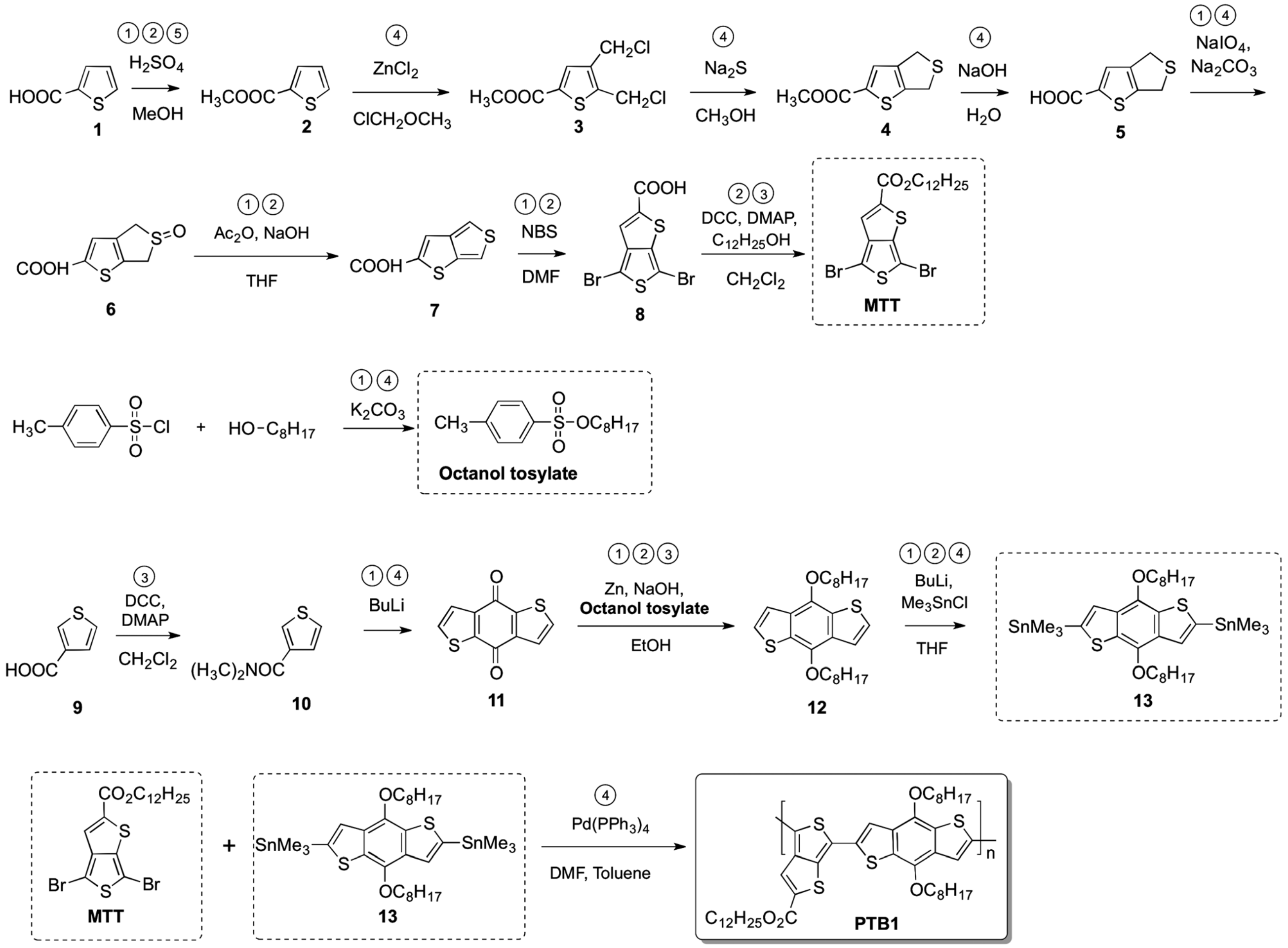
4 **Recrystallization.** We assume 1 g product needs 100 mL solvent and that the procedure is performed only once.

5 **Distillation/sublimation.** We assume no solvent or chemical waste; only energy input.

The requirement for a workup or purification procedure following a synthetic step is indicated by a circled number (corresponding to one of the procedures described above) in Schemes 1–3.



Scheme 2 Synthesis of **P3HT**. Circled numbers represent specific workup procedures, as described in the text.



Scheme 3 Synthesis of **PTB1**. Circled numbers represent specific workup procedures, as described in the text.

We note that an implicit assumption of this framework is that the quantities of materials required for workup will scale linearly, from the gram-scale to scale of thousands-of-kilograms. This may not necessarily be valid, however. Optimization of the synthetic routes and of the process chemistry at the plant-level may enable considerable economies of scale. For example, there may be opportunities for multiple steps to be combined together to reduce the number of explicit isolation steps ("telescoping").[6] Additionally, solvents may be recycled and reused for parts of synthetic procedures. On this basis, we may regard our cost calculations, with and without the inclusion of costs associated with workup/purification, to provide "worst" and "best"-case scenarios, respectively, for the large-scale production of OPV active materials. Ideally, all of the synthetic steps would be collapsible into a single reaction with minimal costs for workup and purification. In contrast, a procedure with little potential for optimization may, in the worst case scenario, be subject to our full estimate for the cost of required workup and purification procedures.

Cost model

For each synthetic step, the quantities of input materials (reagents and solvents) and the reaction yield were identified in order to build a model for the synthesis of each molecule. Additionally, the material inputs required to execute each of

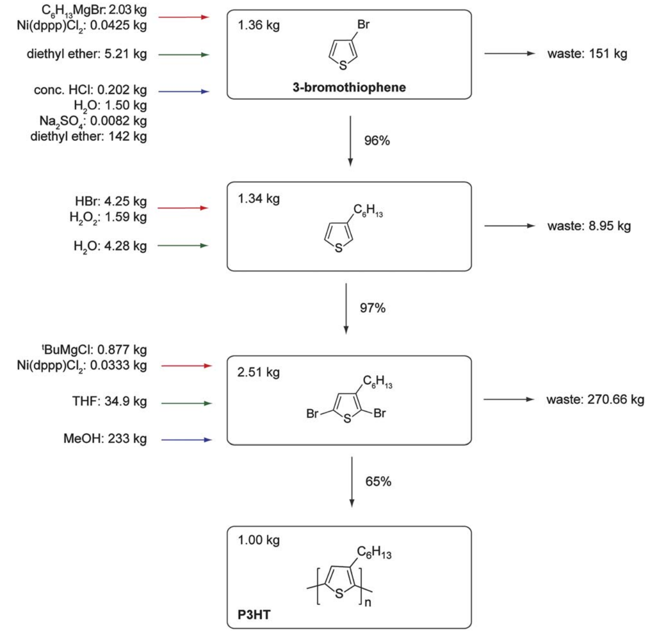


Fig. 2 Flowchart describing the synthesis of 1 kg of **P3HT**. The requisite quantities of reagent (red arrow), solvents (green arrow) and work-up materials (blue arrow) are indicated for each step.

indicated workup and purification procedures contribute to these models. We then calculate the quantities of each input material needed in order to produce a given quantity of product. As an example, our model for the synthesis of **P3HT** is represented graphically as a flowchart in Fig. 2. The first box in the flowchart represents the starting material, 3-bromothiophene. Red arrows indicate reagents, green arrows indicate solvents and blue arrows indicate additional materials required for workup. The indicated quantities of input materials and waste are calculated to produce a kilogram of product. Flowcharts describing the synthesis of the other molecules shown in Fig. 1 are available in the ESI.†

To determine the material costs, we created a database of quotes from major chemical suppliers for each of the materials used in the synthetic procedures investigated herein (see ESI†). For each step, the input material prices were multiplied by the required quantity to determine the material cost. The sum of each of the input material costs for each step was then calculated to determine the total material cost of the entire procedure. This quantity was calculated for cases that both include and exclude workup/purification costs (the "worst" and "best"-case scenarios).

An important assumption of this model is that the prices for these starting materials, reagents and solvents will remain invariant to fluctuations in their supply and demand. A considerable reduction in raw material costs, however, may result from a major industrial effort to scale the production of particular OPV materials, as will be discussed later. We also note that the material costs that we consider represent only one component of the overall cost to produce these materials. In the case of pharmaceutical drugs, for example, materials only account for 20–45% of the cost of drug synthesis. The balance includes contributions for labor, capital, utilities, maintenance, waste treatment, taxes, insurance, and various overhead charges.[6]

Results and discussion

Cost-per-gram as a function of synthetic complexity

The results from our models for each synthetic procedure are summarized in Table 2. Note that calculations are presented for two possible synthetic routes of **PDPP3T**. These routes are described in the ESI.† From Table 2, a clear trend is evident of increasing cost-per-gram (C_g) with increasing synthetic complexity (number of steps). This applies to the scenario that includes our scaled workup/purification procedures as well as the "best"-case scenario in which the workup procedures are omitted. These trends are plotted in Fig. 3. The linear fits to the data (solid lines going through (0,0) data point) reveal slopes of 6.39 $ per gram step and 31.00 $ per gram step for the best (Adj. R-squared = 0.72) and worst-case (Adj. R-squared = 0.91) scenarios, respectively. We note that, although these fits faithfully represent the trend of increasing cost with increasing complexity, they overestimate the costs that are predicted for the simplest molecules such as **CuPc** and **P3HT**.

Cost-per-peak-Watt as a function of OPV efficiency

We note that several studies have investigated the overall cost breakdown for specific organic solar cell technologies including

Table 2 Survey of calculated chemical synthesis costs for several OPV active layer materials

Compound	References	Steps	Reagents [$ per g]	Solvent [$ per g]	Workup [$ per g]	Total (no w/u) [$ per g]	Total [$ per g]
CuPc	7	1	0.13	0.63	0.02	0.76	0.78
Alq3	32	1	0.44	0.00	3.90	0.44	4.34
SQ	14,21	2	3.45	2.42	5.53	5.87	11.39
P3HT	33–35	3	1.72	1.83	12.62	3.56	16.18
DBP	36	3	7.24	0.63	81.72	7.88	89.60
PDPP3T (1)	16,37–41	6	11.89	3.05	149.52	14.95	164.46
PDPP3T (2)	16,37–40,42	6	9.78	2.56	150.91	12.34	163.25
DTS	8,42–44	8	106.02	4.80	41.00	110.82	151.82
PBDTTPD	10,11,28,29,45,46	10	70.97	14.94	361.92	85.90	447.83
PTB1	26–29	14	24.80	43.66	369.71	68.47	438.18

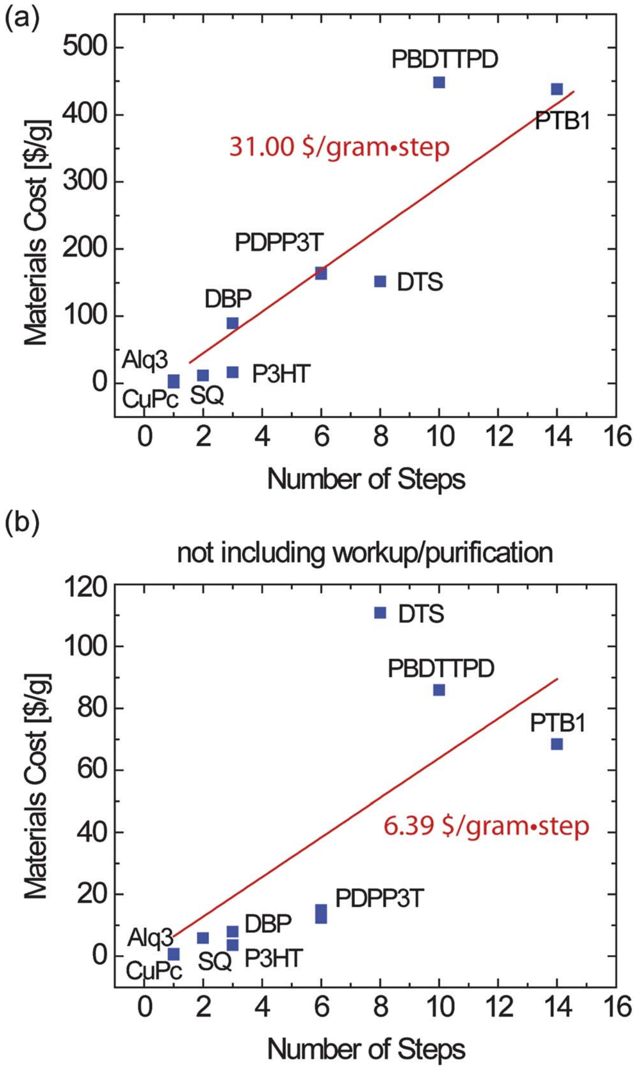


Fig. 3 Scatter plot of the calculated material cost ($ per g) *versus* the number of required synthetic steps (a) including and (b) not including estimated workup/purification costs. See text for details of these calculations. Red line is a linear fit to the data.

structures based on **CuPc**[25] and various polythiophenes.[47–50] The OPV active materials were found to contribute 5–10% of the materials cost for **P3HT**/PCBM structures[50] and 10–20% for **CuPc**/C60 structures.[25] In both cases, the dominant component of the materials cost was identified to be the substrate and transparent conducting oxide (TCO). We also note that, in addition to the cost of materials themselves, an important consideration is the cost of processing these materials into the various layers that constitute the OPV structure. Sufficiently fast and inexpensive manufacturing techniques will be critical to achieving commercial viability, as discussed by Krebs *et al.*[47,49]

Here, we restrict our attention specifically to the contribution of the active donor material to the ultimate solar cell cost in order to assess the impact that synthetic accessibility has on commercial viability. Specifically, we investigate how the scaling of the material cost with synthetic complexity would affect the cost-per-peak-Watt ($ per W_p, denoted here as C_W) of an archetypal OPV structure. To be an attractive material for OPV, the cost contribution of an organic donor material should be much less than the total cost of the OPV module. For example, we may consider the case of CdTe, for which the active layer material cost contributes in the range of 1–10% of the module cost[51] and silicon, in which the active material cost contributes 15–20% of the module cost.[52] For the active layer material cost to be truly regarded as negligible, we identify an active layer material cost target to be 1% of the module cost. For reference, we also consider a more relaxed target of 10% of the module cost. With these targets, and assuming a target module cost of 0.50 $ per W_p,[53] the individual active layer material price should ideally be less than 0.005 or 0.050 $ per W_p. We consider a cell in which the thickness of the donor material (t) is 100 nm, and in which the density of the donor material, ρ, is 1.1 g cm^{-3}.[54] We

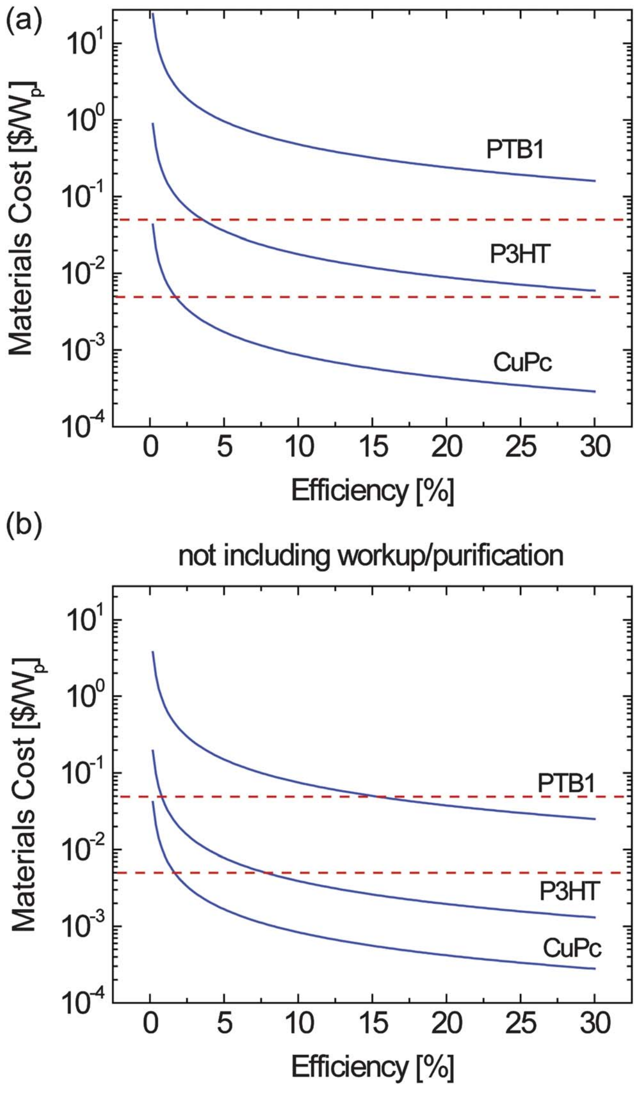


Fig. 4 Calculated material cost-per-peak-Watt ($ per W_p) as a function of solar cell efficiency for hypothetical devices incorporating **CuPc**, **P3HT** and **PTB1**. (a) Includes the cost of reagents, solvents and work-up procedures. (b) Includes only the cost of reagents and solvents. The red dashed lines indicate 0.005 and 0.050-dollars-per-peak-Watt.

assume that the wastage of material during processing at scale is negligible. We calculate the C_W using the following equation:

$$C_W = (C_g \times \rho \times t)/(\eta \times I)$$

here, η is the efficiency of the solar cell, C_g is cost-per-gram and I is the solar insolation under peak conditions, assumed to be 1000 W m^{-2}. Resulting curves for C_W as a function of solar cell efficiency are shown in Fig. 4. Here we only consider **CuPc**, **P3HT** and **PTB1**, as representatives of molecules with varying synthetic complexity (1, 3 and 14 steps, respectively). In the worst-case scenario, in which the material costs include scaled estimates for workup/purification procedures, we find that only the simplest molecule, **CuPc**, will contribute a cost of less than 0.005 \$ per W$_p$, assuming that the OPV PCE is greater than 1.8%. In the best-case scenario, in which workup/purification costs are assumed to be optimized to zero, we find that both **CuPc** and **P3HT** will meet this criteria provided that solar cell efficiencies of 1.8% and 8.0% can be achieved, respectively. We note that in both scenarios the most complex molecule, **PTB1**, fails to reach this threshold, even for PCEs as high as 30%. Plots of C_W as a function of solar cell efficiency for **SQ**, **Alq3**, **DBP**, **DTS**, **PDPP3T** and **PBDTTPD** are shown in the ESI.† Among these, only **Alq3** is calculated to present a negligible cost in the worst-case scenario ($C_W < 0.005$ \$ per W$_p$ when $\eta > 9.6\%$). In the best-case scenario, the costs of the simplest molecules including **Alq3** (1 step), **SQ** (2 steps) and **DBP** (3 steps) would become negligible provided efficiencies of 1%, 13% and 17.4%, respectively. Again, however, the molecules requiring the most complex synthetic procedures, **PDPP3T** (6 steps), **DTS** (8 steps) and **PBDTTPD** (10 steps), would represent a considerable fraction of the OPV module cost ($C_W > 0.005$ \$ per W$_p$). These results suggest that consideration of synthetic accessibility with regard to OPV active layer materials may be critical to achieving an inexpensive and scalable OPV technology. Additionally, these results emphasize the importance of optimizing the process chemistry of these synthetic procedures to minimize the use of reagent and solvent, as well as the number of individual synthetic steps. Based on the cases considered here in the best-case scenario, only molecules with fewer than 6 synthetic steps are found to represent a small component to the cost of a hypothetical OPV module.

One important driver in this analysis is the amount of material required to realize an OPV module. Here, a single-junction effective donor thickness of 100 nm was assumed. Different device architectures, however, may require more or less material, thus affecting cost. In a multijunction OPV architecture, for example, donor and acceptor materials would be needed for each sub-cell in the stack. This would effectively multiply the OPV active layer material costs by the number of sub-cells.

An additional driver that might alter the outcome of this analysis is scale. As mentioned previously, a critical assumption is that prices for starting materials, reagents and solvents will remain invariant to fluctuations in their supply and demand. Sufficient economies of scale, however, may enable considerable price reductions for input materials. As an example, we may consider the case of **CuPc**, which is produced at the scale of millions of kg-per-year. **CuPc** may presently be purchased in bulk from a major chemical company for less than 0.10 \$ per g, or approximately an order of magnitude less than the cost calculated here in our best-case scenario. This suggests a significant economic advantage to industrial synthesis at a very large scale, which may make the commercial outlook for molecules like those considered in this study much more favorable. It is unclear at this time, however, how economies of scale might affect the cost of more complicated molecules.

Summary

We presented a cost analysis for the synthesis of several promising OPV active layers by quantifying material costs of their published small-scale synthetic routes. The material cost in dollars-per-gram (\$ per g) is found to linearly increase with the number of synthetic steps required to produce each material. By estimating the cost-per-peak-Watt (\$ per W$_p$) as a function of power conversion efficiency of an archetypal OPV structure, we find that only relatively simple molecules (<6 synthetic steps) will contribute negligibly to the cost of an OPV module. The synthesis of **P3HT** (consisting of 3 synthetic steps), for example, is found to contribute a cost of 0.004 to 0.02 \$ per W$_p$, given an OPV PCE of 10%. In contrast, **PTB1** (14 synthetic steps) contributes costs of 0.075 to 0.48 \$ per W$_p$. Our findings suggest that the commercial viability of an OPV technology may critically depend on the synthetic complexity of its constituent active layer materials, although economies of scale will likely improve the commercial outlook for these materials. Additionally, this work stresses the importance of optimizing synthetic routes to minimize solvent and reagent usage as well as minimizing the number of required workup procedures.

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