Material Strategies to Accelerate OPV Technology Toward a GW Technology

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With the rise of the solar power century, photovoltaic applications and installations will go beyond the traditional green field power plants and enter any aspect of daily life. Organic photovoltaics (OPVs) demonstrate certified cell efficiencies of over 17% and are expected to contribute to versatile applications powered by solar energy, for instance, applications rely on flexibility, transparency, color management, or integrability. In this work, the progress of OPV technology is briefly reviewed and the material strategies to accelerate OPV technology toward a GW era are analyzed. In addition to the exciting efficiency values achieved for small area devices, there are many important criteria deciding the success of OPV technology. By taking into consideration the synthetic complexity of OPV materials and the operational stability of OPV devices, the industrial figure of merit (i-FoM) is proposed as a fast and reliable method to verify the true potential of a novel material. Furthermore, “soft” key performance indicators are introduced, such as toxicity, flexibility, transparency, processing, which require different development strategies to reflect the potential of OPV technology for specific applications.

1. Introduction

In agreement with the forecasts by international energy portals like the international energy agency (IEA), more than 600 GWp of photovoltaic (PV) modules had been installed by the end of 2019, compared to about 500 GWp worldwide installations in 2018. The IEA predicts solar PV to become the dominant technology driver for the renewable energy turnaround. By today, the worldwide peak capacity of solar energy production has caught up with wind power, and is expected to be the first renewable energy to exceed the TWp limit in the next few years, probably already by 2023.[8] Solar Power Europe reports leverized cost of electricity (LCOE) for photovoltaic power to range from 5 c (kWh)−1 in the North of Europe like in Helsinki and 3 c (kWh)−1 in the south of Europe, like in Malaga, which will further go down to 3 c (kWh)−1 respectively 1c (kWh)−1.[8] Fraunhofer ISE reports in the 2019 PV report that photovoltaic installations are dominated by crystalline silicon (c-Si) with a market share of over 95% in solar farms and on rooftops.[8] With the rise of the solar power century, photovoltaic applications and installations will go beyond the traditional green field power plants and enter every aspect of our daily life. Urban, naval and space mobility, residential buildings and business towers, all types of facades, portable and Internet of Things (IoT) applications, clothing—almost any aspect of our life can and will be powered by solar energy. While c-Si appears untouchable as leading PV main stream technology for a longer time, many of the new applications which rely on flexibility, transparency, color management, integrability or simply elegant appearance require novel photovoltaic materials and technologies.

2. OPV Progress

Organic photovoltaics (OPV), like other thin film PV technologies, is not yet part of this global TW scenario. The first OPV products were launched in 2008/2009 for portable chargers at an efficiency of about 2% and based on a semiconductor blend consisting of P3HT:PCBM.[4] Despite the rather low performance, these first products already showed the characteristic “OPV features” like flexibility, transparency and color variability.[8] An early, very impressive milestone was demonstrated for the organic technology, only 5 years after industrial developments had started—organic photovoltaic modules passed the stability tests according to the thin film IEC 61646 protocols in independent testing by TÜV Rheinland.[8] Since then, the OPV community has concentrated on developing novel material systems for higher efficiency—a development which was outstandingly successful. In the last 10 years, organic solar cell performance was increased from about 8% in 2009 to about 17% in 2019.
The certified record efficiencies beyond 17% were all achieved with non-fullerene acceptors (NFAs). Certified module efficiencies are typically lagging behind the certified cell efficiencies for two reasons: the 1) Geometrical Fill Factor (GFF) and 2) reduced losses for ultra-small active areas. Modules have fundamental optical losses caused by the interconnection areas, which are photovoltaically inactive as they provide low ohmic electrical connection between the single cells. A series connection is typically preferred to keep current densities and the related resistive power losses as low as possible. However, the regime where the top electrode of one cell connects to the bottom electrode of the adjacent cell is photovoltaically inactive. The GFF for larger modules is well approximated by the width of the cell \( w_c \) divided by the width of the cell \( w_c \) plus the width of the interconnect \( w_i \) (GFF \( \approx \frac{w_c}{w_c + w_i} \)). Note that the number of interconnects is one less than the number of cells which has to be corrected for smaller modules. Bus bars or packaging rims are frequently disregarded when calculating the GFF explaining the frequently slightly higher recorded GFF for academic modules when compared to industrial modules. Geometrical Fill Factors (GFF) of over 90% and up to 98% were achieved for specific organic PV module architectures by femtosecond laser patterning. Alternative interconnection architectures are outlining a good compromise between record GFF values and a probably easier to scale “one step interconnect” (OSI) process. But even with industrial ns laser patterning, GFFs of more than 90% are obtained for large area modules. As such, one would expect to see an active area module performance which is coming close to the one of 1 cm\(^2\) cell efficiencies and total area module performances which are not far away from that value for larger modules.

Many record efficiencies are reported for cell areas smaller than 0.1 cm\(^2\). Specific ohmic as well as electronic losses, mainly related to transparent electrodes but also to the device geometry, can be reduced for very small areas. However, losses related to these phenomena are inevitable when going to larger areas like 1 cm\(^2\) in particular due to a tradeoff between conductivity and transparency for the transparent electrode. The current certified record efficiency listed in the solar cell efficiency tables (Progress in Photovoltaics) reports 13.45%, though other institutes reported certificates of over 16% for 1 cm\(^2\) OPV cells. We want to emphasize the importance of certifying solar cells with 1 cm\(^2\) active areas, as these values are expected to hold when scaling to larger areas. Technologically even more important than cell efficiencies are module efficiencies. After a long period of stagnation, new OPV efficiency records were published in 2019 and 2020. The highest certified performance values by today are 12.6% for modules with a total area of about 26 cm\(^2\) (active area efficiency was 13.2%), while modules with about 200 cm\(^2\) active area achieved a total area efficiency of...
11.7% (Figure 1b). At such high performance OPV is on par with the amorphous silicon technology (single as well as multi-junction). Scaling the module area from 26 cm² to over 200 cm² reduced performance from 12.6% to 11.7%, which was more related to coating inhomogeneity rather than to further fundamental loss mechanisms. This again underlines our previous statement on the importance of 1 cm² reports and certificates instead of reports on smaller areas.

Major progress could as well come from introducing alternative standardized ways of reporting performance progress. For several decades, solar cell efficiency progress is reported biannually in the “Solar cell efficiency tables” by Martin Green et al.[19,20] and in NREL’s “Best research-cell efficiency chart.”[13] These tables are effectively tracking progress in technologies like Si or 2nd, and 3rd generation photovoltaic technologies, but often lack the necessary level of detail due to confidentiality, IP issues or industrial strategies. For the R&D community, this means that one gets informed on the progress in respected fields; however, the confidential nature of certificates does cause a discussion on their value for the academic community as learning are not necessarily guaranteed. We therefore strongly support the concept of open access databases, which summarize the most reliable and reproducible information from peer reviewed publications, as an additional standard for reporting solar cell progress. As long as certain quality standards are maintained, we believe that peer reviewed publications can provide information with sufficient precision, in parallel to offering the advantage of full transparency. A corresponding initiative on reporting emerging photovoltaics based on peer reviewed publications is currently under preparation and will go online in late 2020 under “emerging-pv.org.”

Figure 1c summarizes the certified efficiencies for different cell and module areas. As each table reflects the state of the art at a specific point of time, it is important to understand the dynamics behind. Certificates on 1 cm² are typically more than 1 year behind the small area certificates, and module certificates are again more than a year behind the 1 cm² certificates, if a material system is scalable. Following this logic, one would expect to see module certificates with over 15% efficiency within the next 1–2 years. A major, currently not well understood, drop in efficiency from 12% to about 5% occurs between record modules and industrially available modules. That performance drop is not caused by physical limitations, but is rather due to stability issues or the constraints of environmentally compatible industrial printing, which many of the recent record materials do not fulfill. This point will be analyzed in more detail at the end of this perspective.

All current record efficiencies are held with NFAs, which are molecular acceptors with an extended electron system and alternating electron deficient/electron rich units. Besides fullerene based acceptors (FAs), NFAs have proven to be the second major category of acceptor materials for organic bulk-heterojunction solar cells. A possibly third class of acceptor materials—polymeric acceptors—are blooming at the technology horizon, but are not yet at the same level as FAs or NFAs.[24]

The FAs era had identified two physical limitations which prevented organic solar cells from overcoming the 15% efficiency milestone. Primarily, the excitonic nature of organic semiconductors in combination with the formation of low energetic charge transfer states (CT) at the interface between the donor and acceptor were identified to limit the maximum achievable performance, both contributing about 300 mV in Voc losses.[22,23] The Voc related losses of 0.6 V seemed insurmountable for quite a long time.[24] With the emergence of NFAs, that picture changed in two essential points. NFAs exhibit three orders in magnitude higher electroluminescence quantum efficiencies as compared to FAs, $10^{-3}$ instead of $10^{-6}$, reducing the non-radiative Voc losses from 0.4 V for PCBM to about 0.17 V for a NFA.[15] The interface energetics of these systems is no longer dominated by charge transfer states but rather by molecular hybrid states of the acceptor.[25,26] Carrier generation as well as carrier recombination is fundamentally altered in many NFA systems where the HOMO level of the acceptor is energetically matched to the HOMO level of the donor. As charge generation is slowing down for well-matched energy levels, the singlet exciton lifetime starts to determine the external quantum efficiency (EQE). An unprecedented large single exciton lifetime was reported for selected NFA systems, which enabled to reduce non-radiative Voc losses to a minimum while still maintaining high EQE values. It is important to mention that the absence of CT states as well as long singlet exciton lifetimes is not impossible for FAs. An exciton lifetime on the order of 1 ns was measured for PCBM thin films,[28] which is comparable to the one of the high efficiency NFA 9G[27] and hybridized interface states were reported as well for fullerene–polymer blends.[29] A prerequisite to both is the sufficient alignment of the donor’s and acceptor’s HOMO levels. This selection rule clearly favors acceptor systems with an easy to tune HOMO level, which is a major advantage of NFAs over FAs. The potential to reduce Voc losses in NFA-based composites was most impressively demonstrated by Cao et al.[15] who reported non-radiative losses as low as 0.18 V for a semiconductor composite with an ECT energy of about 1.4 eV (Figure 1e).

Despite some fundamental limitations like rather low radiative recombination that currently limits the electroluminescence quantum efficiency of efficient OPV composites to about $10^{-4}$ and the corresponding non-radiative Voc losses to about 0.2 eV, scientists as well as technology experts predict OPV to break through the important 20% efficiency milestone in the next 2–3 years. The significantly higher absorption coefficient of the NFAs in combination with relatively high radiative recombination and the possibility to perfectly match the HOMO energy levels of the donor and acceptor predetermine NFAs to achieve that milestone at first.

One major unique selling point of OPV is the possibility to design not only semi-transparent devices, but instead design devices which are selectively transparent in the visible regime between 400–650 (or 380–700 nm), that is, where the eye is most sensitive. Lunt et al calculated the theoretical limit for energy conversion for visibly fully transparent devices and found a maximum theoretical efficiency of slightly above 20% for devices which do not absorb in the human eye sensitive wavelength regime.[10,11] The excitonic nature of organic semiconductors, which can limit the width of the primary absorption peak typically to 300 nm,[30] makes it possible to design semiconductors which harvest near IR light, while being semi-transparent for the visible part of the spectrum. Electricity-generating windows
are one of the highly topical concepts that excite people’s imagination. The steady-growing European window market with more than 60 million window units sold per year offers a footprint area of about 100 Mio m$^2$ for a transparent photovoltaic technology, which translates into a hypothetical annual capacity of up to 10 GWp installations in buildings only. This is about the size of the total European photovoltaics market in 2018. Based on these figures it appears obvious that semi-transparent or transparent photovoltaics will become an emerging market opportunity for photovoltaics. A recent, very visionary, directive of the European Commission (“Directive 2010/31/EU on the energy performance of buildings”) regulating the energy performance of buildings already proposes all new buildings to be nearly zero-energy by the end of 2020. By harvesting only UV or NIR light, a PV window can almost offer comparable electricity-generations potential as rooftop solar, while it may in parallel provide additional functionalities like peak shifting, advanced shading or even sophisticated autonomous thermal management to enhance the efficiency of buildings.\textsuperscript{[33]} OPV has a clear competitive advantage for transparent PV applications due to its unique excitonic absorption features, and, recent research progress reported solution processed and semitransparent organic solar cells with efficiencies up to 11%.\textsuperscript{[34–36]} The development of semitransparent organic photovoltaic devices is summarized in Figure 1d, listing data from more than 200 reports. An average visual transparency (AVT) of >50% at efficiencies of 8–10% is regarded as a major breakthrough which could trigger the development of a novel generation of photovoltaic products for window integration.

3. Analysis

Despite the recent NFA enabled progress of OPV, one should not expect grid-connected OPV as an application within reach. The competition with other PV technologies, above all crystalline silicon PV, is held in the units of LCOE and measured in c (kWh)$^{-1}$. LCOE depends critically on the lifetime and costs of the installation. Today’s OPV modules are targeting lifetimes of >5 years for flexible products and >10 years for glass-based products, which is contradicting the ambitions to enter the photovoltaics window market where lifetimes beyond 20 years are required. Based on the precise knowledge of efficiency, bill-of-module (BOM) and LCOE is giving enough directivity for driving a technology toward market readiness. However, it is a wide spread misunderstanding that the BOM and LCOE concept can be easily used to direct materials research. First, it is difficult to anticipate the true costs of a material based on early synthesis reports. Second, we are missing the material-structure correlations allowing to predict lifetime only based on the knowledge of a structure. Third, a central pillar of the total material costs is the yield of a process. All these unknown but important factors limit the use of the BOM and LCOE concept for directing material development.

We therefore enter this discussion with a short review on current material costs, before moving over to introducing the synthetic complexity (SC) as a sound alternative to better direct the development of cost efficient and performing semiconductors. Some of the semiconducting materials used in OPV are potentially low cost, and several groups predicted that the BOM costs can be reduced from about 1–10 €/Wp today to less than 0.1 €/Wp at very large production scales at the GW level.\textsuperscript{[37,38]} However, the current generation of materials for record efficiencies represent a step backward in economic efficiency. McCulloch et al. already reported the significant higher synthetic chemical complexity of NFAs versus FAs.\textsuperscript{[39]} The synthetic complexity for the OSC materials was introduced by Po et al. and balances several factors impacting the cost of a synthetic compound.\textsuperscript{[40]} Five normalized parameters are multiplied by weights and added into the synthetic complexity SC, including 1) the number of synthetic steps (NSS), 2) the recrystallization yields (RY), 3) the number of unit operations (NUO), 4) the number of column chromatography (NCC) required for purification and 5) the number of hazardous chemicals used for their preparation (NHC). The SC is calculated according to the following equation. Despite various degrees of freedom to choose the normalization weights, the SC is becoming a standard in reporting of the cost structure of novel materials.

\[
SC = \frac{NSS}{NCC_{\text{max}}} + 25 \frac{\log(RY)}{\log(RY_{\text{max}})} + 15 \frac{NUO}{NUO_{\text{max}}} + 10 \frac{NHC}{NHC_{\text{max}}} \quad (1)
\]

We have analyzed the SC for several of the top performing material classes. Figure 2a compares the synthetic complexity of P3HT and PCBM with some of the most efficient organic semiconductors for OPV like PBDB-T-2F and Y6. One can immediately recognize that the SC of polymers has increased by a factor of more than seven and by a factor of more than three for NFA over PCBM. Even more dramatic is the comparison of various BHJ composites by plotting SC versus PCE (Figure 2b). PFOBT4T-2OD:PCBM, a composite with a complex microstructure arrangement and a maximum efficiency of over 10% has a three times lower SC than PBDB-T:Z2F:Y6. It almost seems that each increase in efficiency was taken at the cost of an increase in SC. We believe that this is an unhealthy trend which needs to be addressed by focusing more research activities on reproducible and easy to scale materials for OPV. Reporting record efficiencies is one essential aspect to illustrate progress in OPV science. Reporting high performing cells and modules from economically scalable and green materials is illustrating progress in OPV technology. We are well aware that it is necessary to upscale materials toward the 100s of gram or even kilogram batch size to get a better understanding on the true materials costs. This is a costly adventure and, as it is a matter of cost, industry has done this only for a limited number of carefully selected OPV materials like P3HT (by Riecke, BASF and Merck), PCBM (from Nano-C, Solenne BV, ...), DPP derivatives (by BASF), PV2000 from Raynergy Tek or the OPV46-X series from Merck. However, the academic community can accompany and ease the scale up. The SC index is as a cost efficient method to compare the expected material costs at an early stage of research. Developing low SC synthetic routes for top performing materials will accelerate the identification of scalable materials.

The full assessment of a PV technology requires detailed know-how on the lifetime of the corresponding solar cells. As
mentioned in the beginning, traditional photovoltaics is compared at the hand of two key performance indicators – €/W_p and LCOE. €/W_p is calculated by dividing BOM/m^2 with the peak power/m^2 and is as such area independent.

\[
\left[ \frac{\epsilon}{W_p} \right] = \left[ \frac{\epsilon}{m^2} \right] / \left\{ A M 1.5 \left[ W_0 \text{m}^2 \times \eta \% \right] \right\}
\] (2)

In difference, LCOE, in its most simplified version, takes into account the lifetime of modules by balancing the total costs spent over the total energy produced within the lifetime span of the module, where r is the discount rate. One recognizes immediately, that n, the lifetime of the system, is becoming the most influential parameter.

\[
\text{LCOE} = \sum_{i=1}^{n} \text{Investment Costs (i)} \left[ \frac{\epsilon}{a} \right] + \text{Operation Costs (i)} \left[ \frac{\epsilon}{a} \right] \div \left( 1 + r \right)^i
\]

(3)

Organic semiconducting materials can be intrinsically stable under long term illumination. Selective candidates for solution processed as well as vacuum processed BHJ composites were reported to be stable for 10 000(s) of hours under AM 1.5 simulated illumination. Most interestingly, such stable performance was reported for solution processed polymer and for vacuum processed molecular BHJ composites as well as for single junction and tandem junction architectures.\(^{[41–44]}\) An ultimate demonstration that OPV can be stable was given by Burlingame et al. who extrapolated an operational T80 (80% of its initial PCE) lifetime of over 27 000 years from accelerated degradation measurements.\(^{[44]}\)

While such thermally evaporated small molecules can be prepared and processed with extremely high purity and precise morphology, which also allows highly stable OLED products, solution processed organic solar cells typically suffer from reduced purity and lower morphological control. Such effects regularly cause burn-in degradation, which often stabilizes after a few hundred hours, but may still lead to about 20 years of predicted stabilized lifetime for example in PCDTBT:PCBM based solar cells (Figure 3b).\(^{[45]}\) With the introduction of non-fullerene acceptors, stability investigations started again from the scratch. Many known degradation mechanisms, as for instance diffusion controlled burn-in effects or interface instabilities leading to vertical phase segregation in fullerene based composites had to be re-examined and re-evaluated. Nevertheless, several NFAs were quickly identified to address limitations.
of fullerene-based acceptors. For instance, IDTBR was recently shown to have strongly reduced burn-in degradation, and, like PCBM based materials, was proven to have an at least identically high potential for long term intrinsic materials stability (Figure 3a).

Even if individual materials are identified to be intrinsically stable enough for decades of operation, it still needs BHJ microstructure optimization, well defined impurity threshold levels, stable interfaces and of course a reproducible processing to reach its full stability potential in a photovoltaic application. Effective approaches to stabilize morphology by improving miscibility, using high Tg materials or adding stabilizing additives (Figure 3d) have been reported by several groups, making morphology one of the best understood stability challenges. While impurities have also been identified as a potential Achilles heel of organic solar cells early on, for each new material system and each stress condition, different interactions may occur. For example the processing additive 1 8-diodooctane (DIO) may cause dramatic degradation in some ITIC and fullerene based systems, while it has little effect on IDTBR based solar cells (Figure 3f).

Consequently, impurities and additives have to be reevaluated and optimized for each system. In a similar fashion, interface layers that can be highly stable in many cases, like ZnO, may cause severe degradation in other materials (Figure 3e). Currently several of such systems which are optimized for morphology, impurities and interfaces exist for well-studied OPV materials with about 3–5% efficiency. However, a similar progress on understanding degradation processes has to be achieved for high performing materials. Elucidating and resolving single degradation processes typically takes years for a novel material. Such long research periods are due to the enormous complexity of degradation phenomena. Lifetime testing is frequently dismissed as something which is too technical and ideally should be done by industry. However, we believe that resolving material instabilities or degradation processes reflects major progress in the science and technology of a research field and therefore should be disseminated in appropriate quality journals. The scientific and technological community has taken great benefit from the bimonthly reported “Solar cell efficiency tables” and from NREL’s “Best research-cell efficiency chart.” One would wish to see a similar effort by reporting “Best research-cell lifetime chart.” For this purpose, it may be necessary to establish institutions.
to measure the lifetime of a photovoltaic research-cell certified. But even without collecting lifetime certificates, the consistent and continuous collection and reporting of lifetimes from peer-reviewed publications would already constitute a major service to the community. The recently founded consortium “emerging-pv.org” is making an attempt to set up such a database with lifetime reports on emerging PV materials.

In summary, the major challenge nowadays is to engineer materials and architectures for OPV products utilizing novel high performance materials with efficiencies above 15% in combination with outstandingly long operational lifetimes. This challenge is at least as important if not even more important than to meet the 20% milestone.

We finalize the analysis of the traditional performance parameters, efficiency, lifetime and costs, for NFA-based composites by summarizing that NFAs have a higher efficiency potential compared to the current generation of FA-based composites, which mainly suffer from insufficient energy level matching and the inherent lower absorption of fullerenes. On the other hand, well performing NFAs have a significantly increased synthetic chemical complexity suggesting that their material costs will be higher than for FAs. Interestingly, environmental stability of NFAs and FAs seems comparable. Both material classes are prone to distinct degradation processes; however, numerous reports demonstrate that NFAs as well as FA-based solar cells can be long-time stable. There are many other important criteria deciding on the success of a photovoltaic product. Many of these criteria are called “soft criteria,” as not all of them can be measured in threshold numbers. Applications to power IoT devices will require a completely different set of key performance indicators (KPIs) as for instance semi-transparent OPV modules for agricultural “double-harvesting” photovoltaics. Figure 4a depicts toxicity and recyclability, flexibility in high yield processing as well as integrability and system compatibility together with color management, homogenious appearance and transparency as further KPI which will decide on the product groups OPV will be able to address. Some of these properties can be easily accessed quantitatively, like transparency (AVT) or color (color rendering index—CRI), while other criteria requiring to meet a yes/no threshold are probably better described quantitatively (flexibility, integrability, recyclability, etc.). A strength/weakness analysis appears therefore as an appropriate method to try a holistic comparison of a novel material’s potential. The discussion of these KPIs, although based on the comparison between FAs and NFAs for OPV, is suggested to be helpful for any new semiconducting material for photovoltaics. We give both acceptors, FAs and NFAs, very good chances to equally address many of the soft KPI for photovoltaics. NFA are somewhat superior in terms of color management; however, PC_{60}BM, a strong UV absorber with reduced absorption in the VIS, has a rather small impact on the color management and/or transparency. Consequently, FAs and NFAs require different classes of donors. FAs require low bandgap donors to cover the VIS and NIR parts of the solar spectrum, whereas NFAs can handle wide bandgap as well as low bandgap donors equally well. Toxicity, recycling, and integrability appear quite comparable for the time being, although extensive clinical studies on non-fullerene acceptors are missing. Toxicity studies on pristine C_{60} reported no acute or sub-acute toxicity in a large variety of living organisms. The situation is not as clear for substituted fullerenes, as some of the C_{60} derivatives were found to be highly toxic. Most of the organic semiconductors have energetic levels suitable for singlet oxygen sensitization, whereas NFAs can be sensitized with VIS or even NIR light as well. A similar situation exists when looking at green solvents. Both, FA- and NFA-based BHJ composites have been reported to be compatible with processing from non-halogenated solvents like tetrahydrofuran (THF), xylene, anisole or mesitylene blends, however, in most of the cases at the costs of reduced efficiency or lifetime.

Figure 4b summarizes the properties of FA- and NFA-based solar cells, denoting industrial competitive and product ready performance with (++), promising but yet not product ready performance with (+) and non-competitive performance with (−). One possibility to read Figure 4b is the observation that both, FAs and NFAs, appear to be very comparable, probably even more comparable than the current publication trends may suggest. Both materials appear to be fairly strong on the “soft” KPIs, but exhibit clear weaknesses in two of the three key performance parameters, namely lifetime and costs for the most efficient material systems. This should be understood as strong motivation to foster research on efficient and stable OPV materials with low SC. A first step in this direction would require efforts toward more regular reporting of lifetime and SC properties of high performance materials. One option to standardize such combined efficiency, lifetime and costs consideration could be the i-FOM (industrial figure of merit), which was specifically introduced as a more balanced way to report the relevant performance of novel material composites.

\[
i-FOM = \frac{\text{PCE} \times \text{Stability}, \text{after } 200 \text{ h}, 1 \text{ sun, arbitrary T}}{\text{SC}}
\]

The definition of the i-FOM is to some extent arbitrary and was chosen such to provide low experimental barriers for the comparison of emerging materials. It is not yet defined as a value allowing prediction of product readiness for a material composite. However, the i-FOM can be discussed as a material’s version of the inverse LCOE. It balances cost \( \times \) lifetime (representing the kWh which can be produced with a given semiconductor over the synthetic complexity SC (representing the costs in € for a given semiconductor composite). Unfortunately, there is only a handful of manuscripts reporting i-FOM values (Table S3, Supporting Information). With more data coming along, an adaption of the i-FOM to more precisely representing the product potential of a material composite appears to become possible. Introducing light accelerated photostability testing in combination with elevated temperature (i.e., 65 or 85 °C) and dedicated weights for the single factors might establish the i-FOM concept as a fast and reliable method to verify the true potential of a novel material. One recent outcome of an extensive i-FOM analysis of NFAs identified the development of NFAs with optimized performance for P3HT as a most promising objective to accelerate the OPV roadmap.
accelerating the OPV roadmap would require to fine tune the material research strategy by finding a better balance between exploring novel materials on the one hand and identifying candidates which are worthwhile for upscaling on the other hand. We believe that these two research directions can be synergistically linked. Extending the materials research strategy to industrial scalable materials would merely require to systematically collect extended material and device information on promising candidates according to their research stage. A reasonable R&D stage definition for OPV composites has to include the following classifications, starting with 1) materials and device research and then proceeding to 2) processing development, 3) prototyping, 4) piloting, and finally 5) upscaling. Depending on the stage of research, the level of technology complexity has to be increased. The transition from glovebox processing to ambient processing as well as the transition from spin coating to a printing method triggers the development of the Processing phase. Prototyping requires the transition from cells to modules, while piloting further requires to exclusively work with non-toxic materials (solvents as well as active materials) and printed top electrodes. Between the individual research stages, performance related gates control whether a material is mature enough to transit into the next stage. The gates need to monitor efficiency, lifetime as well as synthetic complexity or BOM of all layers. This will prevent the progress of expensive semiconductor or unstable interface materials to higher research stages. The detailed gate parameters need to respect the desired product properties. A PV energy harvesting element for IoT applications will require very different gate definitions as a semi-transparent PV window. The concept of this stage gate process is summarized in Figure 4c. The logics behind Figure 4c is based on the observation, that many high potential material systems failed because of a severe drop in either of the KPIs when using ambient processing conditions, green solvents or printed top electrodes in a module configuration. We strongly believe that this concept is applicable and beneficial to all emerging photovoltaic technologies that can rely on a broad and manifold material base, like organic, dye sensitized, perovskite or quantum dot technologies.

4. Summary

OPV has made tremendous progress during the last years. The rise of NFAs has allowed to increase the efficiency to over
17%, and it appears to be only a question of “when” the 20% milestone will be overcome. Despite of the steadily increasing number of exciting new materials, OPV is still struggling to enter the mass market. The discrepancy between record cells and modules and commercially available modules has steadily increased over the last years. On the one hand, this is due to the material development strategy, which has not paid enough attention to stability and costs, but on the other hand, to processing, which has neglected the development of innovative and scalable concepts for green and all-layer-printed modules. By today, the fundamental differences between NFAs and FAs are still subtle—one clear advantage is the strong absorbance of NFAs together with an easy to tune HOMO level, which enabled this significant progress in reducing Voc losses and enhancing efficiency. The operational lifetime of NFA- and FA-based devices so far has not revealed fundamental differences, although one would expect that the strongly suppressed diffusion of NFA will allow to engineer more stable microstructures with reduced requirements for post-processing. The higher efficiency of NFA-based solar cells does not immediately compensate the significantly higher synthetic complexity. However, the chemical versatility of NFA offers this enormous potential for multi-objective optimization and makes it likely that NFA can become the enabling material class to resolve performance, costs, and stability within one material. Advanced material strategy concepts like i-FOM or the stage-gate process are essential cornerstones to accompany and direct these development efforts.

Supporting Information

Supporting Information is available from the Wiley Online Library or from the author.

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Conflict of Interest

The authors declare no conflict of interest.

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