Enhancing the Performance and Stability of Organic Photovoltaics: Design of New Organic Semiconductors for High-Efficiency Solar Cells

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Abstract- ***This study focuses on how to improve performance and stability of organic photovoltaics (OPVs), specifically the new organic semiconductors for high-efficiency solar cells an assessment of the importance of OPVs as cost-effective, light-weight, flexible alternatives to traditional silicon-based solar cells for next-generation renewable energy solutions, addressing the critical challenges of efficiency and stability that currently limit widespread implementation; an overview of conceptual approaches to improve OPV performance, including new molecular designs to enhance light absorption, charge generation and energy conversion; an assessment of the importance of high-performance donor-acceptor materials to promote efficient exciton dissociation, reduce recombination losses, and how the morphological control of active layers could help produce nanoscale architectures that facilitate charge carrier mobility and minimize energy loss; the critical issue of stability, including the ability of OPVs to withstand environmental degradation including moisture, oxygen, light, and other environmental stressors; an overview of new materials that will enhance intrinsic stability of OPVs or the methods that could ensure the protection of devices through encapsulation measures that would facilitate long functional lifetimes; the need for improved degradation resistance both external and intrinsic and requirements to attain it, including the use of novel organic semiconductors resistant to degradation as well as effective and efficient encapsulation approaches; a summary of the need for interdisciplinary solutions to existing barriers to unlock the full potential of these 'green' technologies, and how both the molecular design of organic semiconductors and their thermal, morphological, electrochemical, and optical properties are necessary conditions for the advancement of OPVs and sustainable energy solutions.***

Indexed Terms- ***Organic Photovoltaics (OPVs), Organic Semiconductors, Efficiency Enhancement, Charge Transport, Morphology Control, Degradation Resistance***

I. INTRODUCTION

The potential of organic photovoltaics (OPVs) as a new renewable energy technology has attracted much interest, as OPVs can provide low-cost, lightweight, flexible solar cells that could complement or replace traditional silicon solar technologies in some applications, such as portable electronic devices, building integrated photovoltaics, and flexible electronic or optoelectronic devices (Brabec et al. 2020). Since the 1980s, OPVs development started with an understanding of the general electronic properties of organic materials, using some basic light-absorbing organic materials to investigate the possibility of energy conversion of partially purified organic semiconducting materials (Sariciftci et al., 1992). Significant advancements have been made over the years including the power conversion efficiency (PCE) of OPVs where continual device structural design and the gradual design of new OPV materials have been pushing efficiencies beyond 18% in recent years which has made OPV a viable competitive player in the solar innovation arena (Li et al., 2020). Nevertheless, such improvements cannot completely overcome the fundamental limits of OPV technology, and result in high efficiencies or stabilities that enable commercialization and large-scale deployment compared to the solar cell industry benchmark, i.e. silicon solar cells. OPV efficiency has limited due to

an exciton diffusion and charge mobility properties. Excitons, or electron-hole pairs that are formed when organic materials, namely small molecules or conjugated polymers, absorb light, must dissociate into free charges at the donor-acceptor interface to contribute to the current. The short exciton diffusion length of organic semiconductors is very lower than the thickness of active layer which decreased the number of excitons at the donor-acceptor interface and efficiency (Zhou et al., 2019). In addition, the charge carrier (electron and hole) mobility of organic materials is usually much lower as compared to that in inorganic semiconductors that causes charge recombination loss and drop in current output (He et al., 2020). Morphological instability is another important issue that organic materials incorporated into OPVs will phase separate or crystallize during a long time and reduce the stability and the charge transport properties of the devices (Hao et al., 2020). Apart from the efficiency, overcoming the stability of OPVs is still a hurdle for practical applications under outdoor conditions. When exposed to sunlight, moisture, and oxygen, organic materials are liable to undergo photochemical degradation, causing rapid performance degradation (Parker et al, 2021). This advancement in encapsulation methods to reduce environmental degradation has led to commercialization of OPVs; however, long-term operational stability is still not addressed which limits commercial applications of OPVs for countries with extreme climate (Nguyen et al., 2021). In addition to the morphological instability, active materials are also degraded really fast under operational conditions, which restricts the stability and practicality of organic PVs strikingly lower than silicon-based solar cells which are much more stable. Due to these challenges, new semiconductor designs that overcome limitations in both efficiency and stability are urgently required for OPVs. Current materials present a barrier to a range of devices due to the inherent physical properties of the materials leading to poor charge mobility and sensitivity to degradation and underscore the need for theoretical and conceptual exploration of new materials. Next generation device structures; including donor-acceptor polymer blends, molecular semiconductors with enhanced charge transport, and materials with increased photochemical stability, bring the promise of achieving higher performance and improved stability in OPVs (Li et al., 2020; Zhang et al., 2020). Designing these new materials necessitates a better understanding of the underlying physics of charge generation, transport, and recombination, in addition to further development of molecular engineering for organic semiconductors to strengthen their intrinsic stability and photovoltaic performance. This article seeks to present a more systematic approach toward the design of novel organic semiconductors, specifically for OPVs, and to consolidate theoretical models, guiding principles, and hypothetical design approaches into a conceptual framework. Instead of experimental data, it highlighted the important features of molecular design, charge transport mechanisms, and degradation resistance that are fundamental to enhanced OPV performance and stability. The aim of this paper is thus to discuss the models and frameworks which are key for the rational design of materials that may overcome current limitations of OPV technologies and to provide a path toward solving this problem for future OPV materials. Focusing on the theoretical basis and ways of avoiding these limitations, the ongoing challenge of integration OPVs into a clean, sustainable energy generator is exhibited.

II. FUNDAMENTAL PRINCIPLES OF ORGANIC PHOTOVOLTAICS

The conversion of light energy to electrical energy in organic photovoltaics (OPVs) is based on a number of competing photophysical processes beginning with light absorption, which is the process by which organic semiconductors absorb photons, producing excitons (bound electron-hole pairs created by the absorption of light energy by the organic materials that is an important step in OPV performance) (Brabec et al., 2020). The excitons diffuse in the material to the donor-acceptor phase interface where they dissociate, and charge separation is a step to produce free electrons and holes, generated to facilitate the generation of electric current (Zhou et al., 2019). Because excitons have a short diffusion length in organic materials, rendering them unable to reach the interface for charge separation, the effective endpoint of the donor–acceptor junction is a critical design aspect for improving OPV performance (He et al. 2020). After separation, the electrons and holes then need to be transported to their respective electrodes for collection, which is dependent on the charge mobility

of the materials in the device; poor charge transport can produce recombination losses, which limit the efficiency of OPVs overall (Zhang et al., 2020). To realize a high-power conversion efficiency (PCE), the collection of the charges at the electrodes needs to be efficient, minimizing the losses caused by recombination or to inefficient contacting with the electrodes (Li et al., 2020). The donor and acceptor components in OPVs are of key importance for the efficiency of the device; the donor functions as the electron donor whilst the acceptor is the electron acceptor and they need to have complementary energy levels to promote exciton dissociation (Sariciftci et al., 1992). Donor–acceptor blends, which are nanoscale mixtures of these materials, enable charge separation by creating an interfacial area large enough for exciton dissociation, but the balance of donor and acceptor materials must also be finely-tuned to maximize exciton dissociation while minimizing exciton recombination, making careful molecular design a challenge (Hao et al, 2020). The interfacial layers, such as hole transport and the electron transport layer, are also an important factor in improving OPVs as they can increase the charge collection and transport via pathways with minimal losses for charge carriers traveling from the active layer to electrodes (Parker et al., 2021). More fundamentally, the active layer morphology and phase separation are also critical for OPV performance; too much phase separation can lead to large domains (microns scale) of donor or acceptor phases, retarding charge transport and exciton dissociation, while fine control of the morphology can afford optimal electron-hole pair separation thus reducing recombination and maximizing the efficiency of the device (Brabec et al.2020). Among the various physical mechanisms that govern the performance of OPVs are those which, in principle at least, lead to theoretical efficiency limits for the devices; these limits have many parallels to the Shockley–Queisser limit traditionally associated with conventional photovoltaic devices but also lend insight into the theoretical maximum achievable efficiency in OPVs. When the material bandgap is very large or small, it decreases the efficiency of light absorption and charge extraction, placing a limit on these emerging devices (Zhou et al., 2019). The charge carrier mobilities are much lower than in inorganic solar cells, and the exciton diffusion is a limitation. Hence the theoretical maximum efficiency in OPVs is generally lower than in inorganic solar cells. Nevertheless, OPVs have not yet reached their theoretical limits, but recent advances in material design and device architecture are slowly pushing the OPV performance towards a maximum by developing new materials with optimized absorption spectra, charge transport properties and stability that can contribute to increased performance of OPVs that can make them a potential competitor in the renewable energy landscape (Li, L., Tsetseris, L., Sabatini et al. 2020: Zhang et al. 2020) The nature of exciton dissociation, charge transport and stability are already known at a fundamental level, with theoretical models and experimental investigations fine-tuning our understanding and subsequently leading to innovations in material design, morphology optimization and device engineering.

III. CONCEPTUAL STRATEGIES FOR IMPROVING EFFICIENCY

This contribution consists of a brief analysis of one of the main approaches to enhance the efficiency of organic photovoltaics (OPVs), which is the design of new donor–acceptor systems, where the alignment of the donor highest occupied molecular orbital (HOMO) and the acceptor lowest unoccupied molecular orbital (LUMO) is decisive to attaining optimal alignment for efficient charge transfer and exciton dissociation (Li et al., 2020). Molecular engineering can alter, or "tune," the energy of the HOMO-LUMO levels to maximize the energy offset between the two energy levels of the donor and acceptor to facilitate their exciton dissociation that leads to efficient charge separation with less recombination. Second, the selection of narrow and broad bandgap semiconductors plays a crucial role in the light absorption range and efficiency of OPVs (Organic Photovoltaic cells), as narrow bandgap materials are commonly suitable for maximizing the absorption of the solar spectrum (from red to near-infrared region), while broad bandgap materials are appropriate for high-energy photon capture in the ultraviolet to visible range, thus facilitating an effective balance of light absorption and charge transport properties (Zhou et al., 2019). We therefore propose the incorporation of narrow and broad bandgap semiconductors inside a single device in order to extend the range of light harvesting and maximize the overall power conversion efficiency of

OPVs. A third guiding consideration in molecular design involvesπ-extended systems and planarity; planarity affectsπ–π stacking, which is important to enhance charge mobility in the active layer. In OPVs, the higher planarity of the polymer backbone or small molecules can lead to more intensive π–π stacking interactions, which helps to carry charge carriers along the conjugated network and reduce the exciton recombination, leading to higher charge mobility (He et al., 2020). The more planar the molecules, the better the packing, which improves electronic communication at the molecular level resulting in improved charge transport and device efficiency. Theoretical models indicate that to increase the light harvesting and efficiency of organic photovolatics (OPVs), one must utilize materials with high molar absorptivity, which absorb very well in visible to near-infrared (NIR) region of spectrum (Brabec et al., 2020). Increasing the absorption cross-section of organic semiconductors can be achieved by the design of wider conjugation lengths, strong light absorption and high extinction coefficients, thus allowing more photons to be captured to generate more charge carriers. Heavily light-absorbing material, particularly extended π-conjugation, maximizes a solar spectrum absorbed by a high molar absorptivity to improve power conversion efficiency (PCE). Another attractive strategy for optimum performance is energy cascade and gradient strategies, in which multi-component systems are engineered to facilitate directional charge transport in order to improve the efficiency of organic photovoltaics (OPVs). The energy gradients (meaning the energies of each component in these systems) simply must be tailored to ensure that charge separation and transport leads to efficient movement of generated charge carriers toward their respective electrodes. In this approach, heterogeneous energy levels of the components provide a selective charge transport pathway where the full efficiency of charge carriers is clearer and losses by recombination are reduced (Zhang et al., 2020). Charge collection at the electrodes is a major bottleneck for device efficiency, and the use of multi-component blends and/or heterojunctions that create such gradients can improve collection. These strategies, from the careful tuning of donor–acceptor molecular orbitals, the use of narrow and broad bandgap materials, and the incorporation of π-extended systems to improve charge mobility and the molecular design high molar absorptivity materials and energy cascade systems, are all necessary for improving the performance of OPVs to bring the technology closer to its theoretical efficiency limits and improving competitiveness in the renewable energy marketplace.

IV. CONCEPTUAL APPROACHES TO STABILITY ENHANCEMENT

The crucial, intrinsic and stable long-term performance of organic photovoltaics (OPVs) must be realistically realized by conceptual approaches to enhance photostability, thermal & morphologic stability as well as oxidative resistance and thereby accumulate longer operational lifetime under practical conditions. Photostability being one of the big issues, we are working on new semiconductors that do not suffer from photochemical degradation under continuous sunlight but the research is at a very crude stage here as well. In organic materials, photochemical degradation is mainly caused by production of reactive excited states, which causes dissociation of molecular bonds, and ultimately loss of device performance (Parker et al., 2021). In order to prevent this, electron-withdrawing groups can be inserted into the molecular structure to stabilize these excited states, which prevents photodegradation. In this way, the molecular design with electron-withdrawing groups can promote the stability of the excited states, which can lower the reactivity of the material after the absorption of the photon, thus reducing the adverse effect of the photochemical degradation (Zhou et al., 2020). Not only are these changes proven effective at improving the lifespan of the active materials, but they also ensure the performance of OPVs can be maintained over relatively long periods of time when working under simulated sunlight. Apart from photostability, thermal and morphological stability plays an important role in performance over time for OPVs, especially taking into account a realistic operational environment with high temperatures or changing weather. In order to enhance thermal stability, the creation of rigid, non-meltable structures is crucial for avoiding further degradation of the semiconductor materials at elevated temperatures. In the polymer backbone, incorporating rigid linkers or aromatic systems can improve the resistance to thermal motion and phase changes or molecular reorganization that

can promote performance degradation (He et al. Likewise, by creating materials with strong bonding that do not melt or undergo phase transitions will allow the morphology to persist during the lifetime of the device. Finally, core–side chain engineering, in which the side chains of the polymer are minimized and chemically designed to induce robust phase separation of the donor and acceptor domains, is also a very efficient approach to achieve morphologically stable blends. Such a technique guarantees that the phase separation — illumination of good charge transport and exciton dissociation — is regulated so that over time, it does not run the risk of uncontrolled aggregation or crystallization that could prove detrimental to device functioning (Brabec et al., 2020). Another important issue is oxidative resistance that relates to OPV stability due to the fact that the degradation of the active materials is accelerated by the exposure to oxygen which affects the overall efficiency of the solar cells. These models provide a basis for conceptual models on how to minimize oxygen diffusion pathways to improve oxidative resistance, including strategies such as increasing the thickness of protecting layers or by applying encapsulation materials with a low oxygen transmission rate to protect the OSC from oxidative degradation [83]. In addition, the use of molecular caps or oxidation resistant end-groups can substantially enhance the oxidative stability of the OPVs. For example, these end-caps or protective groups can be designed to inhibit oxygen when it penetrates the active layer and lowers the probability of oxidation reaction which is a potential reaction to degrade the material (Zhang et al., 2020). Then, the molecular structures will be designed with stable capping groups or stable end-groups preventing oxidation, which can help make the bulk organic materials used in OPVs more stable against air and moisture with respect to time, thus improving device stability and performance lifetime. Overall, the improvement of OPV stabilities depends on the approaches of photo stabilities, thermal and morphologies stabilities and oxidative resistances. Durability is enhanced with resistant semiconductor design against photochemical degradation, stabilization of the excited states by using electron-withdrawing groups, and thermal stability via rigid, non-fusible structures. Moreover, phase separate as stable as possible based on the innovation of core–side chain engineering and capping groups or molecular bonds to lessen oxidative degradation are the major effort to elongate both the lifetime and stability of organic photovoltaics. Such deep conceptual advances will be essential to address the remaining hurdles of OPV technology in order to secure the sustainable commercial future of organic photovoltaics.

V. COMPUTATIONAL AND THEORETICAL TOOLS FOR SEMICONDUCTOR DESIGN

Computational and theoretical tools are critical to predict and optimize properties of organic semiconductors for use in organic photovoltaics (OPVs) to increase their efficiency and performance and multiple methods including Density Functional Theory (DFT), Time-Dependent DFT (TD-DFT), Molecular Dynamics (MD), and, recently, machine learning (ML) and artificial intelligence (AI) approaches have emerged to provide such insights. As one of the most widely applied quantum mechanical method, DFT allows for the prediction of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels which are essential to understanding charge generation and transport in OPVs. DFT is valuable for the quantification of these energy levels, guiding the design of materials that maximize exciton dissociation and charge transport, which are fundamental to improving power conversion efficiency (Li et al., 2020). In addition, the reorganization energies that describes the energy needed for the system to rearrange after an electron transfer can also be simulated with DFT, more particularly for determining the driving forces for charge transfer in OPVs where smaller reorganization energies are preferred to reduce energy losses and optimize device performance (Zhou et al.2021). While TD-DFT is not capable of predicting the excited state properties, needed to model intriguing properties like optical absorption, which is a whole concern in itself with regards to OPV material light-harvesting ability, it does widen the applicability of DFT [27]. TD-DFT significantly contributes to the accurate calculations of absorption spectra which is essential as the information of absorbed wavelengths could help in designing semiconductors that are able to harvest solar energy widely (Zhang et al., 2020). TD-DFT allows modeling of excited state dynamics including the time evolution

of the system after photoexcitation which is essential to capture exciton formation, energy transfer, and charge separation (key processes necessary for the proper functioning of OPV devices). The ability to predict these properties a priori render TD-DFT indispensable in the design of new materials with optimized optical properties and with high photoconversion efficiencies. Molecular Dynamics (MD) simulations give complementary information about the morphology and inter-chain interactions in organic materials, which are crucial for tailoring the structure of the active layer in OPVs. For example, the molecular dynamics (MD) simulations provide researchers the ability to simulate the behavior of molecules as they continuously interact with one another over time, enabling visualization of donor and acceptor domain phase separation as well as clarify the effects of phase-morphological changes on charge transport and exciton dissociation (He et al., 2020). MD simulations give stable morphology information through dynamic behavior due to different environmental conditions which is also important for the long-term stability of OPVs. Additionally, MD can be immersed with DFT calculations to assist in designing materials with optimized electronic properties and stable morphologies, which can tackle the two major challenges of OPV, which being efficiency and stability. Machine learning (ML) and artificial intelligence (AI) have recently become a powerful approach to speeding up new OPV materials discovery. By acquiring knowledge on a large data base, ML algorithms are well suited to learn the patterns between experimentally known molecular structure and the properties of the material, and to help in the approach and founded design of materials with the desired properties (that is high charge mobility, improved photostability, etc.) prior to the experimental testing (Brabec et al., 2020). Abstract: AI methods, especially deep learning, have demonstrated the capability to predict the performance of OPV materials by learning complicated mappings between complex molecular structures and their photovoltaic efficiency. These data-driven approaches enable researchers to quickly sample the enormous chemical space available for promising OPV materials, resulting in a much more rapid and efficient material discovery process (Zhou et al., 2021). We have seen emerging and exciting conceptual frameworks that combine ML and AI with more traditional computational approaches like DFT and MD to develop next-generation OPV materials having optimal properties that point toward an efficient route for the design of solar cell semiconductors.

VI. INTEGRATION OF CONCEPTS INTO NEXT-GENERATION OPV ARCHITECTURES

Research on organic photovoltaics (OPVs) is guided by source–sink concepts that aim to improve the performance and stability of these devices1 and has resulted in a number of significant advancements, including multi-junction (tandem) OPVs and non-fullerene acceptors (NFAs), which represent encouraging breakthroughs to propel OPV efficiency and application forward2. Multi-junction organic photovoltaics (MJ-OPV) are solutions to this problem, featuring one or more stacks of layers of organic semiconductors with complementarily matched absorption spectra to maximize the light-harvesting over a broader range (Brabec et al., 2020) and therefore enhance power conversion efficiency (PCE) (Brabec et al., 2020). This is possible as single-junction OPVs can only absorb over a limited range of wavelengths, but these and other opto-electronic devices can take advantage of broadband photon absorption. Tandem OPVs, through the stacking of several layers/optimum energy and bandgap values, can overcome the theoretical efficiency advantages of single-junction devices, putting OPVs on a path to compete with conventional silicon based solar cells at an energy conversion performance level. Similarly, non-fullerene acceptors (NFAs) have been new entrants in OPV devices which also serves as a game-changing materials with many advantages as opposed to fullerene-based acceptors including appropriate absorption, lower energy barrier for charge transport and much improved photochemical stability (Zhou et al., 2021). Moreover, the tunable electronic properties of NFAs, such as energy level alignment, can promote exciton dissociation and charge collection at the electrodes, contributing to improved charge carrier transport as with higher efficiency OPVs fabricated by using NFAs (Li et al., 2020). While the OPV efficiency has improved, there are dedicated design compromises which need to be taken up and that too carefully to achieve the optimal performance. A

primary trade-off is efficiency versus stability Though materials optimized for greater efficiency demonstrate relatively better charge transport and light absorption properties when compared to those optimized for stability, the former are not always the most stable upon environmental exposure, such as moisture, oxygen, and UV light (Parker et al., 2021). Meanwhile, more stable materials might give up some of their performance properties, like charge mobility or absorption efficiency, to remain more long-lived. To address this trade-off, a careful design of these materials is necessary that not only maximizes performance in ideal conditions but also preserves their performance in reasonable conditions over time, allowing OPVs to function efficiently for long periods of time and without appreciable degradation. A second important trade-off is processability vs performance. The nature of OPVs requires that the organic materials have to be processed from a solution and this processing should be scalable to achieve meaningful industrial volumes, but still maintains high device performance. On the other hand, the commercial potential of OPVs is hampered by the complicated synthetic or processing conditions which are difficult to scale-up or yield lower device efficiency, which present challenges for the mass production of high-performance materials (Brabec et al.,2020). Researchers aim to be up to the challenge by targeting high performance but easily processes able materials to allow large scale production and cost-effectiveness for commercialization purposes. The key theoretical performance models help us reserve the lifetime, efficiency and environmental durability of OPVs, participating in the design and optimization of OPVs. These models enable researchers to realistically study OPV performance under practical conditions by including elements like temperature and humidity and light exposure. Predictive models for lifetime are especially significant as they are necessary to describe how degradation will occur over time and predict the operational stability of OPVs in various environments (Zhang et al., 2020). These models are useful for identifying potential failure modes and for guiding the development of more stable materials by simulating degradation mechanisms such as photochemical degradation and thermal degradation. In contrast, efficiency models calculate the influence of alterations in device architecture, material properties, and processing conditions on power conversion efficiency. This way, device design can be optimized before experimental fabrication, making these models ideal for saving time and resources. In addition, environmental durability models simulate the interactions of environmental factors on OPV performance and understand and predict the performance of OPVs in different climates and weather, which is critical data needed to inform the design of devices need to be durable at a commercial level. Through the implementation of these models and algorithms into the design pipeline, OPVs can be designed to achieve an enhanced balance of efficiency, stability and lifetime, improving their commercial scalability in the transition to a more renewable energy market. To conclude, the future development of next generation OPV architectures will depend as much on the theoretical frameworks such as multi-junction OPVs and NFAs as they will on rationally applied design trade-offs that balance efficiency, stability, processability and performance. We need predictive theoretical models for lifetime, efficiency and environmental durability to guide material design and to optimize OPV performance for practical implementation, which will aid in the scalability and durability challenges, meanwhile driving OPVs to higher efficiency and commercial targets.

VII. FUTURE DIRECTIONS AND OUTLOOK

Organic photovoltaics (OPVs) offer a promising future, though the challenge of stability under real-world operating conditions still exists, and current materials remain susceptible to degradation processes driven by environmental factors like moisture, oxygen, and UV radiation, indicating that more in-depth investigation of stability mechanisms accompanied by countermeasures directed toward developing materials with innate resistance to such degradation will need to be addressed (Parker et al., 2021). Research in this direction includes studying the interaction of the environmental factors with the chemical structure of organic semiconductors which could lead to their fast degradation, with some successful strategies namely, the introduction of protective layers, encapsulation techniques or usage of new organic semiconductor materials which are able to resist photochemical and/or thermally driven degradation (Zhou et al., 2021). However, the establishment of universal design rules for OPVs still

represents an open challenge; although some materials and device architectures can be consistently high-performing over a reasonably wide set of conditions, the specific nature of each system—including the ultimate combination of donor and acceptor materials, processing conditions used to prepare the films, and subsequent environmental exposure—will still require opted designs for the given application in order to maximize insights. OPVs used in mobile electronics or building-integrated photovoltaics may have specific stability profiles different from what is needed for large-scale utility applications, necessitating system-specific tailoring that guarantees achievement of the performance and durability specifications corresponding to each use case (Li et al., 2020). With an eye to the future, the vision of theoretical material design for OPVs is focused on the connection of experiment-validation pipelines with high-throughput computational modeling, where theoretical predictions for key material properties (e.g., energy levels, charge transport, photostability) are experimentally validated and iterated, thus accelerating how fast theoretical insights can lead to the realization of high-performance materials (Zhou et al., 2021). Accordingly, the corresponding developments of computational methods, e.g. quantum simulations, are of rising importance to help us model the electronic structure, exciton dynamics, and degradation mechanisms of organic semiconductors so that we can design materials with optimal properties and lifetimes prior to synthesis. However, one of the main contributors of this uncertainty are the challenges in accurately modeling the response of large and electronically complex materials such as those for organic photovoltaics, something that quantum simulations, using first-principles atomic scale principles of quantum mechanics, can offer insights into critical electronic properties of (i) the absorption spectra when exposed to light, (ii) charge transfer efficiencies and (iii) ability for the material to singlet/fraction of triplet excitons (Zhang et al., 2020). In addition, artificial intelligence (AI) and machine learning (ML) methods are being employed in the field of OPV to discover the materials more rapidly by discovering the patterns and relationships in the large datasets that would be difficult for a human to identify and thus allowing for rapid screening of novel materials based on their predicted properties (Zhou et al., 2021). Such AI-accelerated methods allow significant reductions in experimental time and cost by rapidly identifying new candidate OPV materials, thereby greatly accelerating the material discovery process compared to traditional trial-and-error experimental methods. The evolution of OPVs is an interdisciplinary pursuit and will require knowledge and techniques from physicists, engineers, and computational chemists. We have to cooperate with physicists to comprehend the basic interaction of light with materials and charge carriers in OPV and to explore how to develop profound information or to control physical interactions to upgrade proficiency and strength. On the other hand, the engineering community contributes significantly to the translation of theoretical advances into practical, broadly adoptable manufacturing methods, providing essential knowledge on materials processing and device fabrication techniques (Brabec et al., 2020). Computational chemists are essential at the intersection of theory and experiment, taking advantage of sophisticated modeling and simulation techniques to predict material behavior and guide the optimization of organic semiconductor molecular formulations, ensuring that new materials are able to satisfy key theoretical and practical performance criteria. Interdisciplinary collaborations of this kind will help align the research agenda towards solving the remaining challenges in OPV development — namely related to efficiency, stability, scalability, and cost. These joint efforts will enable further development of OPVs to be a scaleable and competitive clean energy technology to continue the next chapter of solar. Future directions of OPV research Towards increasing stability under realistic conditions, degradation mechanisms are being explored and once we understand them, system specific design principles can be established, and with this, we are on a good way to an optimal performance integrated with advances in theoretical material design tools that will give the experimental results (in short, we can say that most of the future is the experimental validation of all the theories made till the middle of this century). Advancements in quantum simulations and AI based approaches will fast track the discovery of new materials, while multidisciplinary synergy across diverse fields will make sure that the innovations are successfully translated into effectively deployable products leading to sustainable energy solutions.

CONCLUSION

This research has provided a comprehensive overview of the major theoretical insights into organic photovoltaic (OPV) material design, emphasizing the critical role of molecular structure, energy level alignment, and morphological control in optimizing efficiency and stability. Theoretical models, such as those that predict HOMO–LUMO levels, exciton dissociation, and charge transport, are invaluable tools for guiding the development of new organic semiconductors with tailored properties for OPVs. These models enable the rational design of materials that maximize light absorption, minimize recombination losses, and improve charge carrier mobility, all essential for enhancing power conversion efficiency. Additionally, the integration of advanced computational tools, such as Density Functional Theory (DFT), Time-Dependent DFT (TD-DFT), and Molecular Dynamics (MD), allows researchers to simulate and optimize the electronic and structural properties of materials before synthesis, significantly accelerating the discovery of high-performance candidates. The insights gained from these models are instrumental in refining the design of OPV materials, particularly as we strive to balance efficiency with stability under real-world operating conditions. Conceptual models also play a crucial role in directing both synthetic and applied research. By providing a theoretical framework that guides the selection of donor-acceptor pairs, optimizes the morphology of active layers, and identifies suitable encapsulation strategies, these models help bridge the gap between laboratory discoveries and practical device performance. Theoretical models serve as a guide to avoid the time-consuming trial-and-error approaches that have traditionally slowed material development, offering a faster, more systematic pathway toward identifying promising materials and architectures. Furthermore, these models help ensure that OPVs are not only high-performing but also robust enough to withstand the environmental stresses they will face over their operational lifetimes. In advocating for the role of theory in OPV innovation, it is clear that the integration of theoretical and experimental approaches is essential to driving the next generation of OPV technology. By utilizing theory to inform material design, we can push the boundaries of what is possible in terms of efficiency, stability, and scalability, ultimately advancing OPVs toward becoming a competitive and sustainable energy solution. As computational tools continue to evolve and interdisciplinary collaborations between physicists, chemists, and engineers strengthen, the role of theory will remain central in shaping the future of OPVs and other emerging solar technologies, fostering innovation and accelerating the transition to a cleaner, renewable energy future.

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