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Design and Performance Optimization of Small Molecule Organic Photovoltaic Materials

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Abstract. In this article, researchers have investigated the design and capability optimisation of SMPS with a particular emphasis on increasing the efficiency of power transfer and developing new manufacturing techniques. Nowadays, the PV industry mostly depends on silicon base technique, but it has many advantages such as high cost, low flexibility and great environment impact. By comparison, the structure of small molecular materials is easily duplicated and has a promising future in the field of PV devices. In this paper, this paper present a discussion on how to increase energy conversion efficiency by using SMPS, as well as the high efficiency of all SMPS systems. In addition, this paper also proposes methods and theoretical frameworks for optimizing material structures using experimental design and machine learning. Not only do they contribute to the improvement of material properties, but they also provide significant theory and practice support for developing highly efficient PV devices.

Keywords: Machine Learning; Approximate Bayesian Computing; Molecular Structure Design.

1. Introduction

Currently, PV generation is one of the most popular fields for the research and development of sustainable energy [1, 2]. Currently, however, PV based on silicon based technology is predominantly based on silicon based technologies: high cost, low flexibility, and significant environmental impact. Currently, the main approach to optimization of small molecular materials is to increase energy conversion efficiency and to develop novel techniques for the production of small molecular materials. In this paper, this paper will focus on how small molecular materials can increase the energy conversion efficiency, and the way in which they are treated, as well as discussions on why they are highly effective, experimental and machine-learning techniques are applied to optimise the composition of the equipment and increase the efficiency of the power transfer.

2. Engineering Applications on Small Molecule Photovoltaic Systems and Organic Solar Cells

If the design is suitable, it is possible to significantly improve the optical and electrical characteristics, molecular layout, aggregation, and degradation of the material. They are light weight, cheap, flexible, and compatible with large area printing and fabrication. Thus, they can be widely used in demanufacturing.

3. Experimental Principle

In the process of designing small molecular solar cells, an organic heterostructure is used to prepare a novel small molecule donor ZR1 which has a bigger co-planar nucleus and an extended conjugation length to enhance the transfer of the charge carrier and reduce the conformational chaos. Molecules have been created to obtain polymer flatness and close molecular packaging that allows them to absorb light waves more easily. The optimization of the layered structure, the phase separation and the size of the domain guarantee the high efficiency of the charge transfer and the reduction of the degeneracy.

At the same time, attention should also be paid to the energy loss in the system, The energy loss is expressed as follows:

$$q\Delta V_{OC} = E_g - qV_{OC} = (E_g - qV_{OC}^{SQ}) + (qV_{OC}^{SQ} - qV_{OC}^{rad}) + (qV_{OC}^{rad} - qV_{OC}) \quad (1)$$

$$= \left(E_g - qV_{SQ}^{OC}\right) + qV_{OC}^{rad,belowgap} + qV_{OC}^{non-rad} \quad (2)$$

$$= q\Delta V_1 + q\Delta V_2 + q\Delta V_3 \quad (3)$$

V_{SQ}^{OC} is the maximum open circuit voltage at the SQ limit. $q\Delta V_1$ is an unavoidable loss in any solar cell and depends only on the band gap of the absorber and the conditions at the specific solar spectrum and temperature. This loss is typically determined using the photovoltaic bandgap energy. $q\Delta V_2$ is the additional radiative recombination loss due to absorption below the band gap. In ZR1 and ZR1 In the hybrid system, this loss can be observed through Fourier transform photocurrent spectroscopy (FTPS-EQE) measurements. For the ZR1 hybrid system, due to the large HOMO energy level gap, the sub-bandgap absorption of the charge transfer state (CT) can be clearly seen in the FTPS-EQE spectrum, while ZR1 mixed system shows a smaller HOMO energy level gap, so the loss in this part is smaller. $q\Delta V_3$ is the loss in open circuit voltage caused by non-radiative recombination, measured by electroluminescence quantum efficiency (EQEEL). Increasing EQEEL indicates a reduction in non-radiative recombination losses in the corresponding system. In the table, ZR1The EQEEL is significantly higher than that of the ZR1 mixture, indicating that ZR1 has lower non-radiative recombination losses, thereby improving the open circuit voltage and overall device performance.

The significance of the polymers and small molecules based on benzodithiophenes (BDT) is the achievement of PCE for Organic Photovoltaic (OPV) equipment. BDT-based materials are particularly good at getting past the 10 percent efficiency threshold. In the course of the design, BDT-based skeleton is optimized through the combination of various donor (D-A) combinations to enhance PV properties, extend conjugation and increase charge transfer with π-bridges, and design regular structures to enhance crystallinity and phase separation. Furthermore, the side-chains of the composites have been optimized to increase the solubility, crystallinity, and phase separation of BDT-based materials. Various alkyl chains and substituted positions were investigated to obtain optimum performance. In addition, the addition of electron withdrawing or electron donor groups to BDT can greatly influence the electron and PV properties [3].

4. Experimental Method

4.1. Material Synthesis

The synthesis of the small molecule donorZR1 by the Knoevenagel reaction is more than 70%. Thesynthesis involves long side chains on two-dimensional conjugated thiopheneunits and hexyl-substituted rhodanine terminal acceptors to enhance solubilityand photovoltaic performance. Many kinds of BDT-based polymers and small molecules are synthesized by means of Stille coupling, Suzuki coupling, and directly arylation. The choice of synthetic route depends upon desired functional groups and molecular structure.

4.2. Device Preparation

The ITO/PEDOT/conventional aluminum construction apparatus is composed of ZR1 and an electron-accepter Y6 or IDIC-4Cl, which is produced in chloroform, and is then applied to the base by spin-coating method. Thermal annealing of the films at 120oC for 10 minutes has been shown to improve morphology, and it has been discovered that Thermal annealing is a key step towards maximum photoelectricity conversion efficiency (PCE).

A variety of OPV devices have been developed for small-molecule PV materials, which consist of single layer, double layer and three layer heterojunction structure. Active layers are typically deposited using spin-coating or blade-coating techniques. Optimization of the active layer is accomplished through optimal phase separation and charge transfer through adjustment of donor acceptance ratios, annealing temperatures, and treatment additives.

4.3. Characterization Techniques

For small molecule solar cells, a variety of characterization techniques are used. The absorbance spectra of ZR1, Y6 and IDIC-4Clin are determined by UV Visible Absorbency Spectrometry, which offers information on the Optical Band Gap and Molecule Aggregation in Solid Membrane. Cyclic voltammograms (CV) measure the HOMO and LUMO energy levels for both the donor and the receiver, respectively.

Scanning Wide Angle X Ray Scattering (GIWAXS) has been applied to investigate the properties of the molecules and their packing in the membrane. TEM and resonance soft X ray scattering (RSoXS) have been applied in this paper to investigate the shape of the composite membrane and its phase separation.

J-V characteristics are measured under standard AM 1.5G lighting to evaluate the photovoltaic performance of the device, providing data on open circuit voltage (VOC), short circuit current density (JSC), fill factor (FF) and power conversion efficiency (PCE). External quantum efficiency (EQE) analysis determines the photon-to-electron conversion efficiency at different wavelengths, helping to calculate JSC and understand the spectral response of the device.

For small molecule photovoltaic materials, nuclear magnetic resonance (NMR) spectroscopy is used to confirm the chemical structure of the synthesized material. Gel permeation chromatography (GPC) was used to determine the molecular weight and molecular weight distribution index of the polymer. Measure the optical properties and band gaps of materials using UV-visible absorption spectroscopy. Cyclic voltammetry (CV) is used to determine electrochemical properties and energy levels. Atomic force microscopy (AFM) and transmission electron microscopy (TEM) are used to study the surface morphology and nanoscale phase separation of the active layer. J-V characteristics are measured under standard conditions to evaluate the photovoltaic performance of the device. External quantum efficiency (EQE) analysis to determine spectral response and charge collection efficiency.

5. Data Processing

In order to achieveover-limit efficiency in small molecule organic solar cells by optimizing thehierarchical morphology, a UV-visible absorption spectrometer was employed to analyze the absorption spectra of ZR1, IDIC-4Cl, Y6 in the solution and film.

The J-V characteristics of the apparatus have been tested with a normal AM 1.5 G guide and have been assessed for VOC, short-circuit current density (JSC), FF and PCE. The is calculated by means of an Outer Quantum Efficiency (EQE) measure at various wavelengths for analysis of the PCE conversion efficiency at various wavelengths. The morphology of ZR1 and the mixed membrane were studied by using TEM and RSoXS. The size and phase separation of the first and second phase have been determined in various amplification conditions. Based on the calculation of the purity of the phase, the influence of the phase separation and the morphology of the morphology were analyzed.

In order to study the molecular design of BPV materials, NMR spectra were applied to determine the composition of these compounds. The MW and MW distribution index were measured by GPC. Measurement of optical characteristics, band gaps, and absorption spectra are performed with an UV visible absorption spectrometer. The electrochemical properties and energy levels of materials are measured by cyclic voltammetry (CV). Analyze the oxidation-reduction potential of the donor and recipient molecules with a standard reference electrode and calculate the HOMO and LUMO energy levels.

The morphology and nanometer-scale phase separation of the active layer have been investigated by AFM and TEM. Visualization of the phase and morphology of materials by means of imaging. The J-V properties of the apparatus shall be tested in normal illumination and shall be assessed for VOC, short circuit density, charge coefficient and photo-electric conversion efficiency (PCE). Analysis of the spectrum response and the collection efficiency of the electric field is performed with an EQE measure.

Optimization of the phase separation and charge transfer performance is achieved by regulating the donor/receiver ratio, annealing temperature, and adding agent. Record the photoelectricity property data in various working conditions, and make the optimum condition.

6. Experimental Results and Discussion

The synthesis of Z1 using Asmall molecular donor (2 D: 2 ', 3' -d '] Benzenesulfonyl (DTBDT) is carried out to optimize the hierarchy of the structure in order to obtain a fully small molecular organic solar cell with more than 14% efficiency. ZR1 is a A-π-D-π-A configuration, where DTBDT is used as a donor, and bisthiophene is used as a π bridge to enhance molecular flatness and stiffness [1]. The single-crystal structural analysis of ZR1 indicates that ZR1 is highly planar and tightly packed, with a π-π stacking distance of 3.58 å, which helps to increase the efficiency of hole transportation. Organic solar cells (OSCs) are fabricated with ZR1 as donor and Y6 and IDIC-4Cl as acceptors. Following optimisation, the ZR1 cell has a maximal PCE of 14.34% (PCE certified at 14.1%), while the non-optimised ZR1 cell has a maximum PCE of 9.64% Owing to the donor/receiver ratio and the heat anneal process, the electro-optical properties of the apparatus are greatly improved. The ZR1 system has an open-circuit voltage (VOC) of 0.86 V, a short-loop current density (JSC) of 24,34mC-2, and a charge factor (FF) of 68.44% [4]. The ZR1 has been studied with the method of Transmission Electron Microscope (TEM) and Resonance Soft-X Scattering (RSoXS). It has been shown that these hybrid membranes have optimized hierarchical morphology that facilitate charge separation and transport. In the ZR1 system, the presence of a small phase area of approximately 10 nanometers and an larger primary phase area was observed. This kind of multiscale nanostructure has been shown to be useful in the study of solar cells. The fiber morphology and more homogeneous phase separation structure contribute to the formation of continuous penetration net and increase the efficiency of charge transmission efficiency in ZR1 system by means of grazing incidence wide angle X ray scattering (GIWAXS). It is found that ZR1 has a high degree of aggregation and polycrystal orientation after heat annealing. The π-π stacking peak is located at 1.71 Å − 1, and corresponding π-π stacking distance is 3.67M.

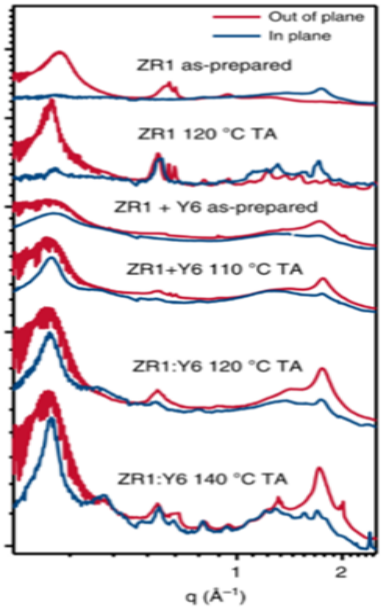

Fig 1. Microstructure of pristine and hybrid films [5].

By applying the Scherrer equation to calculate the crystal coherence length (CCL), the crystallinity of the ZR1 film is significantly improved after thermal annealing (Figure 1). The ZR1 system exhibits low energy loss (E_{loss}), mainly due to the smaller $q\Delta V_2$ (0.04 eV) and higher external quantum efficiency electroluminescence (EQEEL, 1.1 × 10^-4), indicating that the non-radiative recombination loss is relatively small Low ($q\Delta V_3 = 0.24eV$). In contrast, the ZR1 system results in a higher non-radiative energy loss ($q\Delta V_3 = 0.38eV$) due to a larger $q\Delta V_2$ (0.12 eV) and a lower EQEEL (5.0 × 10^-7) (Figure 2 and Figure 3) [5].

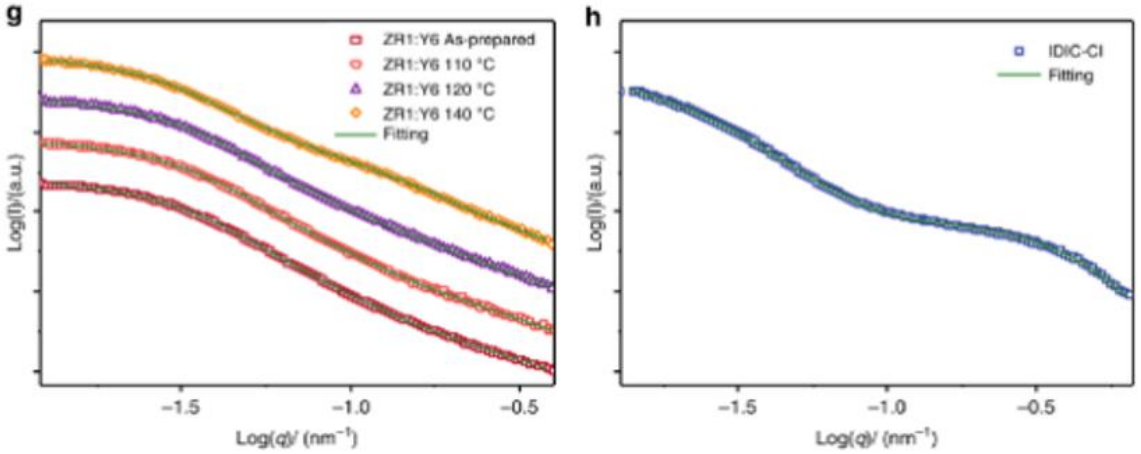

Fig 2. ZR1 and ZR1 Morphology Analysis of Hybrid Films [5].

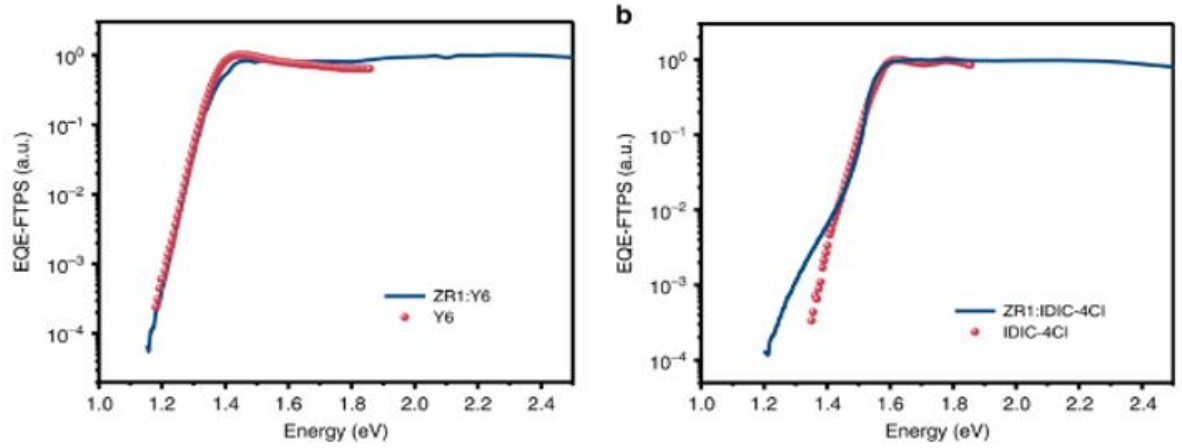

Fig 3. Energy loss quantification [5].

The molecular design of the organic PV materials of benzodithiophenes includes optimizing the structure of the polymer backbone. This process is achieved through different donor-acceptor (D-A) combinations, π bridges, and terpolymer designs. The D-A copolymerization technique has been widely used in recent years as a novel approach for designing highly effective PV polymers. Through selection of a variety of donor and acceptor monomers, it is possible to tune the optical characteristics of the polymer and to optimize its photoelectricity performance.

Inserting π bridges can adjust the conjugated structure of the polymer backbone, thereby optimizing its photovoltaic performance. The introduction of π bridges can increase intermolecular interactions and improve charge transport capabilities. The terpolymer design utilizes the complementary absorption characteristics of various monomers to fully absorb visible light. This design strategy greatly increases the efficiency of the PV system by combining the merits of several monomers.

Optimisation of flexible chains It is possible to optimize the solubility, π-electron transfer and compatibility with the fullerene of a polymer by modifying its length, its form (straight or branched), its location, and its amino groups. Appropriately designed side-chains can improve the workability

and properties of materials. The electron and photoelectricity performance may be significantly influenced by the introduction of electron withdrawing or electron donor groups into a BDT structure. The function replacement can be used to regulate the energy level of the material and the photoelectricity conversion efficiency.

Two dimensional conjugated side-groups are used to improve the PV properties of conjugated polymers. The two-dimensional conjugated structure helps enhance intermolecular π-π stacking and improve charge transfer efficiency. The proposed scheme offers an integrated approach to improve the properties of PV materials, and establishes the basis for high efficiency PV devices.

7. Optimization of Small Molecule Photovoltaic Devices

To increase the energy transfer efficiency of all the little molecules. Based on machine learning, the performance of the system has been greatly improved in recent years [2].

Through the experiment, this paper have optimized the parameters such as the concentration of liquid, the amount of donor, the annealing temperature, and the length of time. Successful design of nano-structured phase separation morphology can facilitate the separation of exciton and enhance the yield of chargecarriers.

In the process optimization, 4 technological parameters are selected: Donor/Acceptor Concentration, Donor/Acceptor Ratio (Donor Fraction), Hot Anneal Temperature, Thermalanneal Time. It should be noted that in the course of the trial, researchers assumed that annealing would have little effect on the results of the experiment. Annealing causes the molecular arrangement in the material to tend to reduce entropy, thereby increasing the material's strength and service life.

Before analyzing the measurement data, filtering is used to exclude abnormal data to avoid deviations in the analysis. Then, variance analysis is carried out on the data to quantize the measured parameters, and the results are optimized with smaller contributions prior to the next step in the optimization of the parameter. Through this series of optimization steps, researchers can determine the optimal process conditions to achieve the preparation of high-efficiency photovoltaic devices (Figure 4).

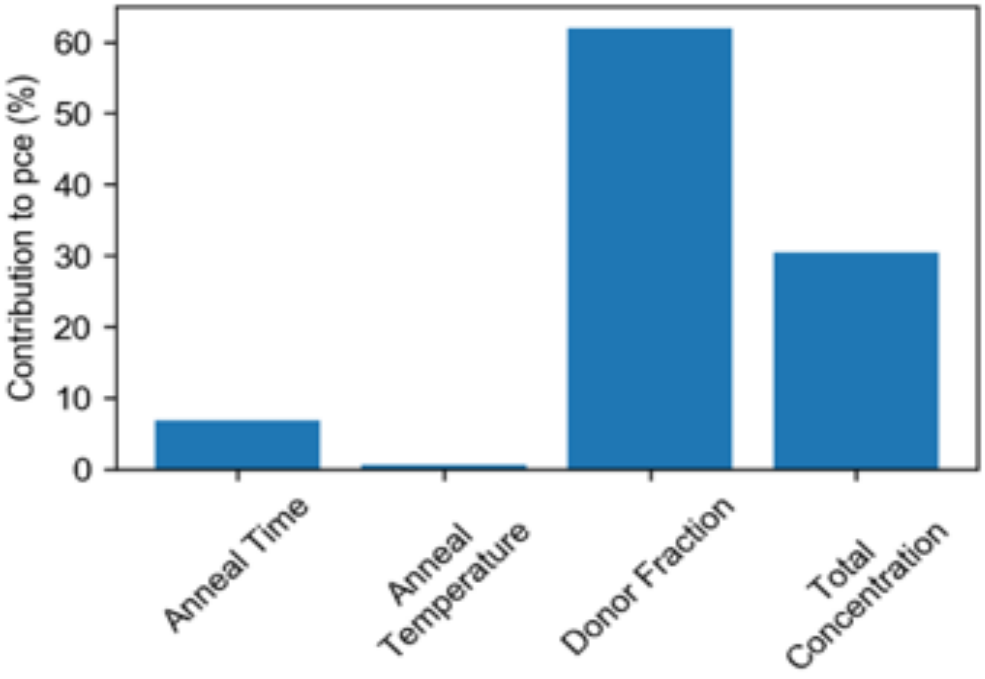

Fig 4. Variance analysis plot of the first round of optimization [2].

After the first round of optimization, the four main parameters were changed to three. It can be found that the PCE of the device is higher at higher annealing temperatures. The first round of optimization will optimize the annealing time

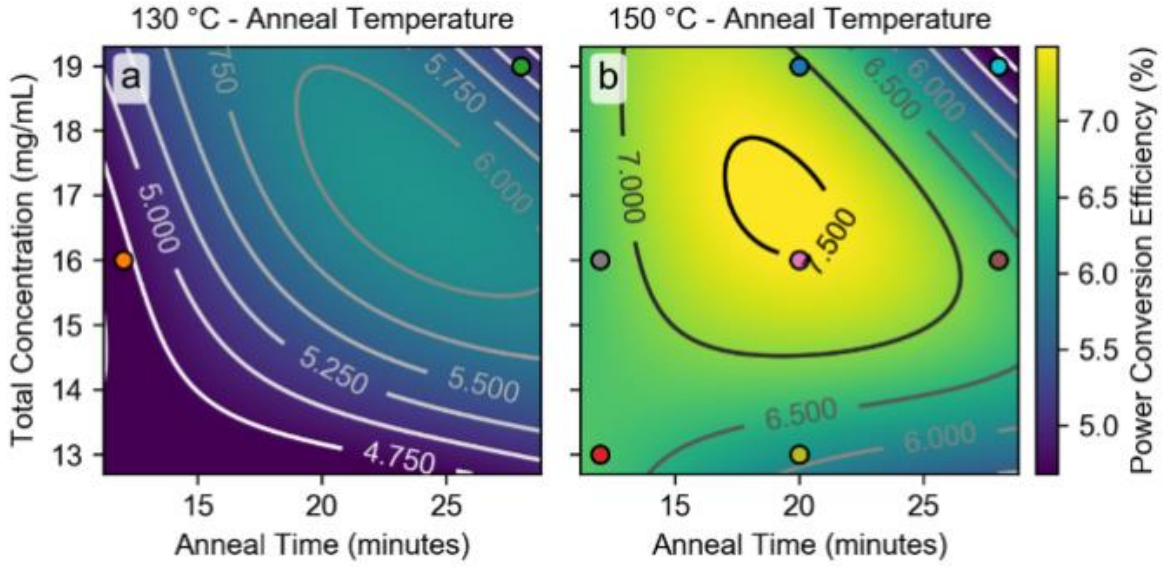

Fig 5. ML-generated PCE maps for the second round of optimization of devices [2].

After performing parameter optimizations through machine learning, the following conclusions can be drawn.

By comparing the two graphs in Figure 5, it is clear that the 150 ° C annealed device has higher efficiency than the 130 ° C annealed device. Based on the PCE variation, it is found that the annealing temperature is the most important factor for PCE, next is annealing time, then total concentration.

Optimization of the forecast method improves the effectiveness by 17 percent. However, this optimization approach also has drawbacks. Due to the small measurement size and no a priori reference for the data, the naive Bayes system cannot be used for prediction [6]. This is one of the disadvantages of machine learning predictions. In order to increase the effectiveness of follow-up investigations, investigators need to look for prior knowledge of the data so that they can be accurately predicted.

8. Future development and discussion

It is true that machine learning can help us optimize the measurement direction and improve it by matching different weights among various parameters. However, due to the small measurement range, the data obtained is small. Using the machine learning framework for prediction may lead to prediction results due to insufficient data volume. Deviation [7].

When making material selection and optimizing molecular structures, it is recommended to use an approximate Bayesian framework for prediction. Before making predictions, the range of measurement parameters should be expanded and refined to obtain more initial parameters. These parameters can be used as prior probabilities to be predicted under an approximate Bayesian framework, which ensures the accuracy of predictions to a certain extent. At the same time, a large amount of data avoids accidental experiments and undesirable local optimal solutions. Through this framework, power conversion efficiency can continue to be improved [8].

9. Conclusion

In this article, this paper investigate the design and performance optimisation of small-molecular organic PV materials, which have been shown to be promising. Such advantages include the fact that PV equipment is light weight, cheap, flexible and suitable for large-scale printing and production. The experiment was carried out by means of UV Visible Absorption Spectrum (UV), Electrochemical Cycle Voltammetric, TEM and Resonance Soft X Ray Scattering (SR).

It is found that optimization of donor acceptance ratio, anneal temperature and time can obviously increase the efficiency of PV conversion. The maximum efficiency of ZR1 is up to 14.34%. Moreover, in the case of the proposed model, the performance of the model can be improved to 17%. However, it is recommended to use an approximate Bayesian framework to expand the range of measured parameters to guarantee prediction accuracy without void experimental chance and poor local optimal solutions. All of these findings will be helpful to develop high efficiency PV devices.

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