Research Progress on the Mechanism of Carrier Rate Enhancement in Organic Semiconductors

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Abstract: Organic semiconductors are one of the key research topics nowadays. The researchers conducted an in-depth exploration of it from multiple aspects, such as materials, performance improvement, and device structure optimization. In recent years, the topic of increasing carrier migration rate, which is related to semiconductor performance, has attracted much attention due to its profound academic and application value. This review summarizes the charge transfer methods, with a focus on several widely applied enhancement strategies such as traditional doping and molecular optimization strategies. While focusing on the strategies for enhancing the carrier migration rate, the application drawbacks of each strategy were also summarized, such as the inherent defects of the dopants themselves and the complexity of the molecular optimization strategies in practical operations. In addition, special attention has been paid to the latest research achievements in optimizing the charge transport performance of semiconductors by applying machine learning at present, closely integrating the research topic with The Times. Finally, this review looks forward to future research on carrier transport in organic materials, hoping to provide a reference for the design optimization of semiconductors in the future.

1 INTRODUCTION

Organic semiconductors, as an emerging material, have been widely applied in multiple fields such as optoelectronic devices and electronic devices since their discovery. It is of inorganic semiconductors have lower cost and better flexible structure design can be higher. However, while organic semiconductors are constantly being developed and applied, their relatively low electrical conductivity has restricted their development. Therefore, the research on enhancing the electrical conductivity of organic semiconductors has attracted widespread attention. The carrier migration rate in organic semiconductors is closely related to their electrical conductivity. Traditional methods for increasing the carrier migration rate include, but are not limited to, doping materials and optimizing the molecular arrangement of organic semiconductors. With the continuous development of machine learning, existing studies have applied machine learning to the improvement of carrier rates in organic semiconductors.

Based on the existing traditional methods for enhancing the carrier migration rate of organic semiconductors, this paper reviews several valuable strategies for improving the carrier migration rate, including doping organic semiconductors, optimizing the molecular arrangement of organic semiconductors, and predicting the carrier migration rate of organic semiconductors through machine learning. It aims to guide future research.

2 DOPING

Doping refers to the introduction of impurity atoms or molecules into organic semiconductors. By altering their energy band structure and increasing the concentration of charge carriers, the electrical conductivity and photoelectric properties of the material can be enhanced, thereby improving the carrier migration rate.

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2.1 Traditional Doping

Traditionally, doping is mainly divided into n-type and p-type doping.

N-type organic semiconductor doping refers to the introduction of impurity atoms or molecules that can provide free electrons into organic semiconductor materials, thereby increasing the concentration of free electrons in the materials and enhancing their electrical conductivity and electron mobility. Based on this principle, researchers have been constantly exploring how to improve the doping efficiency to further enhance the material performance. Ye (2023) found in his research on the design and synthesis of n-type organic semiconductors that enhancing the doping efficiency between dopants and polymers could effectively increase the electrical conductivity of organic thermoelectric materials. The N2200 series of polymers synthesized based on his strategy saw a significant increase in electrical conductivity under N-type doping.

Recently, Zhao et al. (2024) proposed an n-type doping method based on cation exchange. The research found that by selecting the appropriate dopant and ionic liquid, both high doping efficiency and high cation exchange efficiency can be achieved simultaneously, and a high doping level can be obtained, thereby significantly improving the electrical conductivity of electronic devices. The research results show that the cation exchange doping method leads to a significant increase in the electrical conductivity of the samples, and the highest achieved electrical conductivity is 0.01 S cm^{-1}. This confirms that this method has great potential. At the same time, because it is somewhat difficult to select the appropriate dopant and ionic liquid, this method also poses certain challenges in practical operation.

P-type organic semiconductor doping refers to the introduction of impurity atoms or molecules capable of accepting electrons into organic semiconductor materials, thereby generating holes in the materials, increasing the hole concentration, and enhancing their electrical conductivity and hole mobility. By comparing the electrical properties of the device before and after P-type doping, Shan (2023) found that after epitaxy of the F6TCNNQ small molecule on the surface of the DNTT single crystal device, the shift rate increased by nearly double. Ye (2023), while researching to enhance the doping efficiency of N-type semiconductors, found that improving the doping efficiency could also significantly increase the electrical conductivity of P-type doped PDPPT series polymers. It has been confirmed that doping of P-type organic semiconductors can effectively increase the carrier migration rate.

2.2 Contact Doping

When a semiconductor comes into contact with a metal, a potential barrier layer is often formed. However, when the doping concentration of the semiconductor is very high, electrons can pass through the potential barrier through the tunneling effect, thereby forming a low-resistance ohmic contact, which facilitates the transport of charges. Contact doping is an effective way to form ohmic contacts in organic semiconductor devices.

Zhu (2022), when applying contact doping to solve the problem of non-operation of polymer transistors with coplanar structures, deposited molybdenum trioxide as a doping layer at the contact interface between the metal electrode and the semiconductor layer. The research found that the contact doping improved the overall charge transport of the device, thus enabling the device to start working. It can be seen that contact doping is effective in improving the carrier transport of organic semiconductors.

2.3 Photocatalytic Doping

Chemical doping is an effective method to improve the carrier migration rate of organic semiconductors. Compared with the dopants relied on in other chemical doping, the significant selectivity and efficiency of photocatalysts in promoting REDOX reactions have attracted widespread attention. Jin et al. (2024), based on the room-temperature treated solution and by adjusting the light dose to control the doping level, investigated the N-type doping and p-type doping in photocatalysis, as well as the simultaneous n-doping and p-doping, respectively. The experimental results show that the photocatalytic P-type doping of PBTTT increases its electrical conductivity from 10^{-5} S cm^{-1} to more than 700 S cm-1. The photocatalytic n-type doping of BBL makes its electrical conductivity lower than 10^{-5} S cm^{-1} before doping, and increases to nearly 1S cm^{-1} after two minutes of illumination. When N-type doping and p-type doping are carried out simultaneously, the conductivity of p (g42T-T) in photocatalytic p-type doping reaches 200 S cm^{-1}, and the conductivity of BBL in photocatalytic N-type doping reaches 0.1 S cm^{-1}. A series of research results have confirmed that photocatalytic doping can simply and effectively increase the carrier migration rate of organic semiconductors in three cases. This method is fully feasible for the performance optimization of organic semiconductors. This section must be in two columns.

3 MOLECULAR OPTIMIZATION STRATEGY

3.1 Enhance π-π Stacking

Enhancing the intermolecular π-π packing can improve the planarity of molecules, optimize the arrangement of molecules within organic semiconductors, and thereby increase the carrier migration rate of organic semiconductors. The principle is that π-π stacking causes the electron clouds between molecules to overlap each other, thereby enhancing the electron coupling between molecules and improving the carrier transport efficiency between molecules.

Wang (2022) from Nanchang University constructed two polymers with dicyanobenztriazole as the receptor in the experiment. The study found that the polymer with a stronger π-π packing had a higher carrier migration rate. In the subsequent research, three halogen-free ternary donor polymers based on dicyanobenzotriazole were designed, which have a more ordered arrangement, stronger π-π stacking, and also have better charge transport performance. It is evident that the π-π packing between molecules is closely related to the carrier migration.

In addition, there are photoelectric performance test experiments based on triperylene monoimide spiralane molecular films. The results show that the π-π stacking of TNP-6CN films is stronger. The maximum electron mobility of the thin-film device, 1.0×10-3cm^2 V^{-1} s^{-1}, has a better carrier transport capacity than the maximum hole mobility of the TNP-BF thin-film device, which is 5.2×10^{-4}cm^2 V^{-1} s^{-1} (Zhou, 2023). Both of the above experiments show that the tight π-π packing between molecules can effectively improve the carrier migration rate of organic semiconductors.

3.2 High-Speed Spin Coating and High-Temperature Annealing

When dealing with materials, such as single-layer films formed by organic semiconductor materials, the annealing temperature of the film and the spin coating speed are two crucial conditions. When conducting related research, Liu et al. (2024) found that the two external processing conditions, annealing temperature and spin coating speed, like the molecular structure, can directly affect the orientation of specific molecules in the film: Under the conditions of high-temperature annealing and high-speed spin-coating, specific molecules in the film have enhanced lateral orientation. This led to an increase in the carrier migration rate of TCDADI-C16 from 0.01 cm^{2}V^{-1}s^{-1} to 0.05 cm^{2}V^{-1}s^{-1} and that of TCDADI-C24 from 0.13 cm^{2}V^{-1}s^{-1} to 0.20 cm^{2}V^{-1}s^{-1}. Dai (2023) found in the study of DPT-TT that as the annealing temperature gradually increased to 150℃, the carrier migration rate of the device gradually increased. This is also evidence that high-temperature annealing can effectively increase the rate of charge migration.

Unlike directly manipulating the internal structure of molecules, controlling the annealing temperature and spin coating speed to change the molecular orientation based on the external processing conditions of the material, thereby enhancing the carrier migration rate of organic semiconductors, is more operable.

3.3 Side Chain Engineering

Introducing long alkyl chains into polymers can increase their solubility, but intermolecular packing often decreases. The effect of introducing short alkyl chains is exactly the opposite. Although it will reduce the solubility, it will effectively increase the molecular packing, thereby enhancing the carrier migration rate. Side chain engineering is precisely a good method to improve the performance of organic semiconductors by altering the molecular structure by introducing side chains of different groups into the main chain of organic material molecules, either by changing their molecular packing structure to enhance charge transport or by optimizing their energy level structure to increase the carrier migration rate.

Introducing hydrogen bond interactions is a beneficial strategy for sidechain engineering. Chen et al. (2023) synthesized three thiazole side group DPP polymers and confirmed that two of the polymers with hydrogen bond interactions had better aggregation than those without hydrogen bond interactions, thereby having higher carrier migration rates.

Zhao et al. (2025) from Fudan University obtained three derivatives by substituting branched alkyl or alkoxyl groups on the molecules of the y series non-fullerene acceptor materials. After analyzing and comparing the single crystal structures, it was found that after optimizing the crystal packing through side chain engineering, the derivatives were more likely to transfer charges along the π-π direction due to the enhanced π-π packing interaction. Thus, it has a higher carrier migration rate. It once again confirms the feasibility of sidechain engineering as an effective method to increase the carrier migration rate of organic semiconductors.

4 MACHINE LEARNING PREDICTS THE MIGRATION RATE OF ORGANIC SEMICONDUCTORS

The carrier migration rate of organic semiconductors is mainly affected by the molecular packing structure and the charge transfer integral. Machine learning can quickly predict key parameters through modeling. Continuous training and verification of the model can achieve high-speed and accurate prediction of the carrier migration rate.

Johnson et al. (2024) proposed in 2024 to utilize machine learning to predict organic materials with the desired crystallization form through the thermal properties of organic molecules. In its experiment, ML was successfully applied to identify six organic molecules, confirming the feasibility of applying machine learning to the prediction of the thermal properties of organic semiconductors. Because the carrier migration rate of crystalline organic semiconductors is higher than that of amorphous organic semiconductors, the organic molecules with crystalline transformation identified through the ML algorithm in this study not only have excellent thermal properties of high melting point and crystallization driving force, but also have a higher carrier migration rate when applied to semiconductors. It is strong evidence that machine learning can be applied to the improvement of carrier migration rate in organic semiconductors.

Meanwhile, starting from the intrinsic disorder of organic semiconductors, Padula et al. (2025) derived a deep learning combined model based on quantum mechanics and provided a dynamic Monte Carlo prediction for the carrier migration rate using two strategies for evaluating dynamic disorder. It has been confirmed that machine learning can be applied to effectively eliminate the phenomenon of charge carrier localization hindering transport caused by the intrinsic disordered action of organic materials.

The research on high carrier migration rates using machine learning methods is still ongoing. When studying the carrier mobility of organic semiconductors, obtaining the transfer integral of all molecular pairs of organic materials is an indispensable prerequisite step. The team led by Wang (2023) from Tsinghua University has developed a machine learning model based on artificial neural networks to accelerate and predict the transfer integrals of organic semiconductors. This model has effectively predicted the transfer integrals of four typical organic semiconductor molecules in experiments and can be used to explore the relationship between the carrier migration rate of organic semiconductors and temperature. After future improvement, it can also be applied to the study of static disordered organic thin film charge transport. Moreover, when the obtained mobility and the mobility calculated through density functional theory are almost the same in terms of anisotropy and absolute magnitude, the time required for the model's prediction is only one millionth of that required for the calculation. It has been verified that the machine learning method has great application value in exploring the improvement of the carrier migration rate.

5 CONCLUSION

This review focuses on the research of the mechanism for improving the carrier migration rate of organic semiconductors. It reviews and summarizes two widely used strategies for improving the performance of organic semiconductor devices at present, namely, doping and molecular optimization strategies. By emphasizing the analysis of their advantages and outlining their disadvantages, it is convenient for readers to understand the current research status of the carrier rate of organic semiconductors. Meanwhile, it summarizes the new method of applying machine learning methods to predict carrier migration, which is in line with The Times. This is conducive to people studying the improvement of career migration rate while exploring the potential of this field, and flexibly combining and applying new technologies and methods in the era of artificial intelligence, while improving the existing traditional methods. Against the backdrop of the rapid development of information technology, research in the field of organic semiconductors has continuously stimulated cutting-edge exploration and innovation. Research in this field will continuously promote the in-depth integration and development of materials science with other disciplines, injecting vitality into the development of The Times. It is believed that the research perspective on carrier migration in organic semiconductor devices will be broad in the future.

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