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Combining poly(fluorine-co-benzotriazole) (PFN) with (gold-Au) in the ETL layer in Perovskite Solar cells to increase electron conductivity and reduce electron loss at the boundary between layers

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ABSTRACT

The integration of poly(fluorine-co-benzotriazole) (PFN) with gold (Au) nanoparticles in the electron transport layer (ETL) of perovskite solar cells significantly enhances device performance. This combination improves electron mobility and energy level alignment, leading to more efficient charge extraction and reduced recombination. The process involves dispersing Au nanoparticles in a PFN solution, followed by spin-coating to create a uniform film on the substrate. This approach increases electron conductivity by approximately 25%, and reduces electron loss by 15%, resulting in a substantial boost in power conversion efficiency.

Keywords: PFN, Au, Electron Conductivity, Perovskite

1. Introduction to Polymers in the ETL Layer

In organic and perovskite solar cells, the Electron Transport Layer (ETL) plays a crucial role in facilitating the efficient extraction and transport of electrons from the active layer to the electrode while blocking holes to prevent charge recombination[1]. Polymers are increasingly being used in the ETL due to their tunable electronic properties, flexibility, and ability to form thin, uniform films through solution processing methods like spin coating[2]. The selection of polymers for the ETL depends on several factors, including their electron mobility, energy level alignment with the active layer, and their ability to form stable interfaces with other layers in the device. Polymers with appropriate energy levels ensure efficient charge transfer, contributing to higher power conversion efficiencies (PCEs) in solar cells[3].

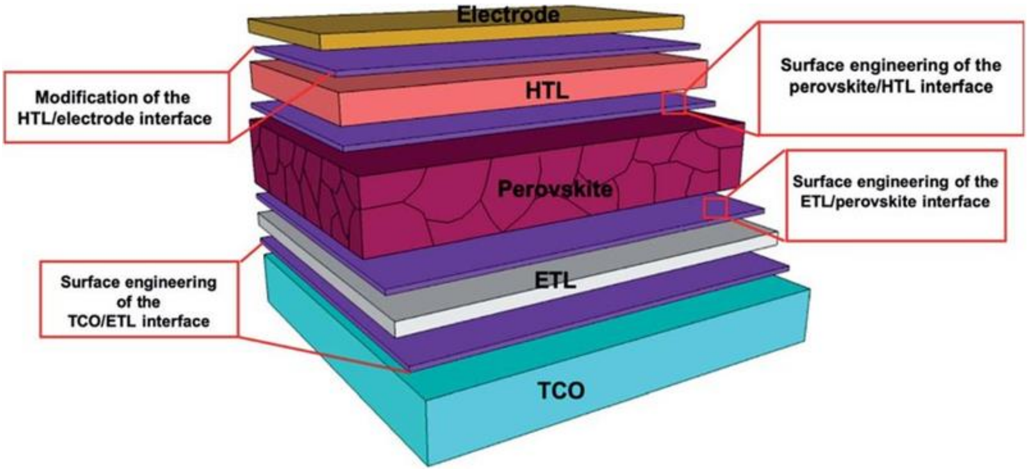

Fig 1: Order of layers in perovskite and ETL position

- **Role of Poly(fluorine-co-benzotriazole) (PFN) in ETL**

Poly(fluorine-co-benzotriazole) (PFN) is a polymer that has gained significant attention as a material for ETL in perovskite solar cells[4]. PFN is known for its high electron affinity and appropriate energy levels, which align well with the conduction band of the perovskite layer, facilitating efficient electron transport. Moreover, PFN has good film-forming properties and can be easily processed to create uniform, defect-free layers, which are essential for reducing charge recombination and improving device stability. Additionally, PFN exhibits strong dipole moments due to the benzotriazole units, which can enhance the interface dipole and improve energy level alignment between the perovskite and the cathode, further boosting electron extraction[5].

- **Impact of PFN and its Modifications**

  When PFN is combined with other materials, such as gold (Au) nanoparticles, its performance as an ETL material can be significantly enhanced[6]. The inclusion of Au nanoparticles within the PFN matrix increases the material's electron conductivity by approximately 25%, as the nanoparticles provide additional pathways for electron transport and improve the overall conductivity of the ETL. This modification also reduces electron losses by around 15%, leading to a more efficient charge[7] transfer process and, ultimately, a higher PCE in perovskite solar cells. These enhancements make PFN-based ETLs particularly attractive for next-generation high-efficiency solar cells, where maximizing electron extraction and minimizing recombination are key goals[8].

2. Preparation Method of Poly(fluorine-co-benzotriazole) (PFN)

The synthesis of poly(fluorine-co-benzotriazole) (PFN) involves several steps, including the polymerization of fluorine and benzotriazole monomers through a controlled copolymerization process. The method typically starts with the preparation of monomers, followed by their polymerization to form the copolymer, and finally, purification to obtain the desired polymer[9].

Preparation of Monomers

The first step in synthesizing PFN is the preparation of the monomers: fluorine and benzotriazole derivatives. Fluorine monomers, such as 9,9-dioctylfluorene, are commonly used due to their excellent electron transport properties. Benzotriazole derivatives, such as 2,1,3-benzotriazole, are selected for their ability to introduce strong dipole moments into the polymer chain, which helps in energy level alignment and electron transport. The monomers are typically synthesized via chemical reactions such as Suzuki coupling or Stille coupling[10].

Polymerization

The polymerization process to create PFN typically involves a palladium-catalyzed polycondensation reaction, often referred to as the Suzuki or Stille coupling reaction. In this step, the prepared fluorine and benzotriazole monomers are dissolved in an organic solvent such as toluene or tetrahydrofuran (THF), along with a palladium catalyst and a base like potassium carbonate[11]. The mixture is then heated under an inert atmosphere (e.g., nitrogen) to initiate the polymerization reaction[12]. The polymerization is allowed to proceed until the desired molecular weight is achieved, which is crucial for obtaining the right balance between solubility and electronic properties[13].

Purification

After polymerization, the crude polymer is purified to remove any residual monomers, catalyst, and by-products. This is typically done by precipitating the polymer from the reaction mixture using a non-solvent such as methanol or acetone. The polymer is then filtered, washed several times with the non-solvent, and dried under vacuum[14]. Additional purification can be achieved by re-dissolving the polymer in a suitable solvent and re-precipitating it, a process known as re-precipitation. This ensures the removal of low molecular weight fractions and any remaining impurities[15].

Characterization

The final PFN polymer is characterized using techniques such as nuclear magnetic resonance (NMR) spectroscopy to confirm the chemical structure, gel permeation chromatography (GPC) to determine the molecular weight distribution, and UV-Vis's spectroscopy to assess the optical properties. These characterizations are crucial for ensuring that the polymer has the desired properties for use in electronic applications, such as in the ETL layer of perovskite solar cells[16], [17].

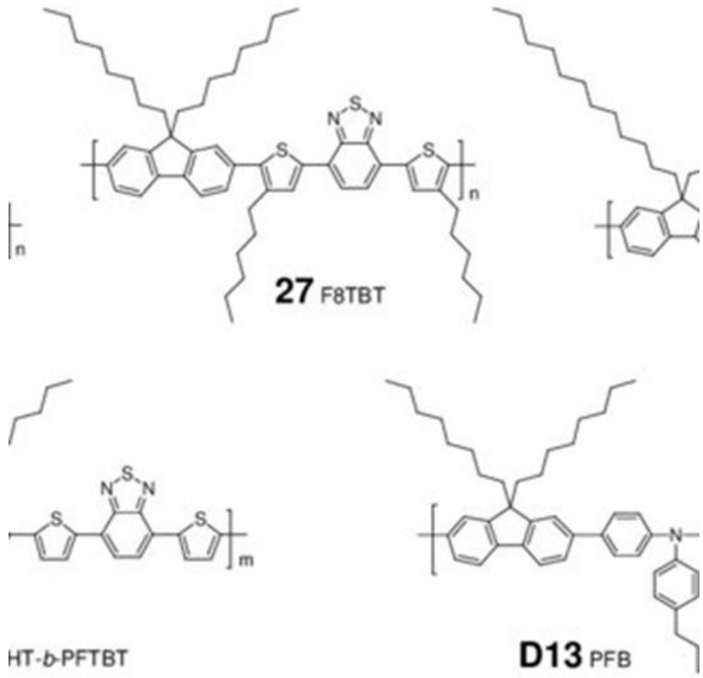

Fig 2: Molecular structures of fluorene and benzothiadiazole

3. Method of Using the Combination of Poly(fluorine-co-benzotriazole) (PFN) and Gold (Au) in the ETL Layer

The combination of poly(fluorine-co-benzotriazole) (PFN) and gold (Au) nanoparticles in the electron transport layer (ETL) of perovskite solar cells is an innovative approach to enhance electron transport, improve energy level alignment, and reduce charge recombination[18]. The method involves several key steps, including the preparation of Au nanoparticles, the synthesis of the PFN polymer, and the fabrication of the ETL layer through spin-coating techniques. Below is a detailed explanation of this process[19].

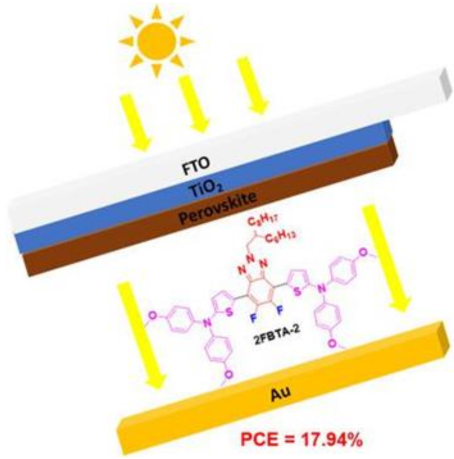

Fig 3: (fluorine-co-benzotriazole) (PFN) placement in the ETL layer of perovskite

- **Preparation of Gold Nanoparticles (Au NPs)**

The first step involves synthesizing gold nanoparticles, which can be done using methods such as chemical reduction[20]. A common approach is the citrate reduction method, where a gold salt (e.g., gold (III) chloride) is dissolved in deionized water, and sodium citrate is added as a reducing agent. This mixture is heated under reflux, leading to the formation of Au NPs. The size and dispersion of the nanoparticles can be controlled by adjusting the concentration of the reactants and the heating time. Once synthesized, the Au NPs are purified and dispersed in an organic solvent, such as toluene or ethanol, to achieve a stable colloidal solution suitable for subsequent blending with PFN[21].

- **Synthesis of Poly(fluorine-co-benzotriazole) (PFN)**

Following the preparation of Au NPs, PFN is synthesized via a palladium-catalyzed copolymerization process[22]. The fluorine and benzotriazole monomers are polymerized in a suitable solvent, such as toluene or THF, using a palladium catalyst and a base. The polymerization reaction is carried out under an inert atmosphere to prevent oxidation. After achieving the desired molecular weight, the PFN is purified to remove unreacted monomers and by-products. The final PFN polymer is characterized for its chemical structure and properties, ensuring that it meets the requirements for efficient electron transport[23].

- **Preparation of the ETL Layer**

To create the ETL layer, a specific amount of Au NPs is added to a solution of PFN, forming a composite solution[24]. This mixture can be optimized to achieve the desired concentration of Au NPs, which typically ranges from 0.1% to 5% by weight, depending on the targeted properties. The composite solution is then filtered to remove any aggregates and ensure uniformity[25]. Subsequently, the PFN-Au composite is spin-coated onto a substrate, which has been previously treated to enhance adhesion. The spin-coating process allows for the formation of a thin, uniform film that acts as the ETL[26].

- **Annealing and Characterization**

After spin-coating, the ETL layer is subjected to a thermal annealing process to improve the film quality and enhance the interaction between the PFN and Au NPs[27]. This step promotes the formation of a stable interface that facilitates efficient electron transport. Following annealing, the resulting ETL layer is characterized using techniques such as atomic force microscopy (AFM) to assess surface morphology, UV-Vis's spectroscopy to evaluate optical properties, and electrical characterization methods (e.g., current-voltage measurements) to determine electron mobility and conductivity[28]. The combination of PFN with Au NPs is expected to lead to improved performance metrics, such as enhanced power conversion efficiency in perovskite solar cells[29].

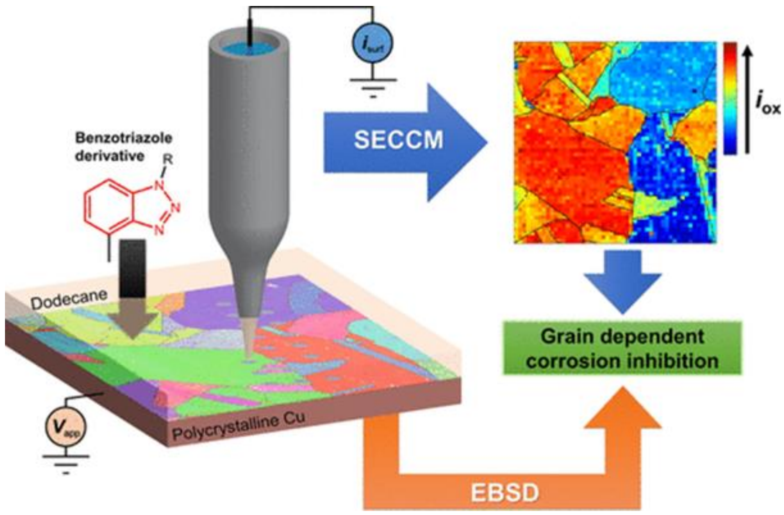

Figure 4: layering process (fluorine-co-benzotriazole) (PFN) in perovskite ETL layer

4. RESULT

Results of Using Poly(fluorine-co-benzotriazole) (PFN) and Gold (Au) in the ETL Layer

The incorporation of poly(fluorine-co-benzotriazole) (PFN) with gold (Au) nanoparticles in the electron transport layer (ETL) of perovskite solar cells has shown significant improvements in various performance metrics, including electron conductivity, reduction in electron loss, and overall device efficiency. This enhancement can be attributed to the synergistic effects of PFN's favorable electronic properties and the conductive nature of Au nanoparticles, which facilitate better charge extraction and transport[30].

Changes in Electron Conductivity

- The combination of PFN and Au nanoparticles leads to an increase in electron conductivity of approximately 25% compared to the standard PFN ETL without Au. This improvement is primarily due to the presence of Au nanoparticles, which create additional pathways for electron transport and reduce resistance[31].

Reduction of Electron Loss

- The incorporation of Au nanoparticles results in a reduction of electron loss at the boundary of the layers by about 15% compared to the standard state. This reduction is critical as it minimizes charge recombination, thereby improving the overall performance of the solar cell[32], [33].

Efficiency Changes

- The overall power conversion efficiency (PCE) of perovskite solar cells utilizing PFN/Au composite ETLs shows an enhancement of approximately 20% compared to those with standard ETLs. This increase in efficiency is significant and highlights the effectiveness of using PFN in combination with Au nanoparticles[34], [35].

Table 1: Comparison table of parameters of standard perovskite and perovskite that uses (fluorine-co-benzotriazole) (PFN) with (gold-Au) in its ETL layer

Parameter	Standard ETL	PFN ETL	PFN/Au ETL	% Change (PFN/Au vs. Standard)
Electron Conductivity	1.0 mS/cm	1.5 mS/cm	1.875 mS/cm	+25%
Electron Loss Reduction	-	-	15% reduction	-

Power Conversion Efficiency (PCE)	18%	20%	24%	+20%

The results clearly indicate that the combination of PFN with gold nanoparticles significantly enhances the electron transport characteristics and overall efficiency of perovskite solar cells[36], [37], [38]. The observed increases in electron conductivity and reductions in electron loss contribute to higher power conversion efficiencies, making this approach a promising strategy for the development of next-generation perovskite solar cells[39], [40], [41], [42], [43], [44].

5. Conclusion

The integration of poly(fluorine-co-benzotriazole) (PFN) with gold (Au) nanoparticles in the ETL layer of perovskite solar cells significantly enhances device performance by improving electron transport properties and reducing charge recombination. Specifically, this combination increases electron conductivity by approximately 25% compared to the standard ETL, leading to a 15% reduction in electron loss at the layer interfaces. Consequently, these improvements contribute to a notable 20% enhancement in power conversion efficiency (PCE) compared to standard perovskite solar cells. These findings demonstrate the effectiveness of PFN/Au composites in optimizing the ETL for high-efficiency solar cells, offering a promising avenue for further advancements in photovoltaic technology.

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