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Tailoring Carbazole derivatives as potential hole-transporting materials for perovskite solar cells: Synthesis, photophysical study, and DFT investigations

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ABSTRACT

The development of ideal hole-transporting materials (HTMs) is crucial for enhancing the performance and stability of perovskite solar cells (PSCs). The HTMs play an important role in extracting holes from the perovskite layer and protecting the perovskite from moisture and other environmental degradation. Here, we are report for the design of six novel carbazole-based donor-acceptor-donor (D-A-D) type HTMs, incorporating linear hexyl and ethyl hexyl chains with electron-withdrawing fluorine and cyano substituents, which can be synthesized through a straightforward synthetic route. Before synthesis, it is essential to do theoretical study to understand the structure-property relationship, which is fundamental for developing highly efficient HTMs. Out of the six designed materials, only one HTM (DCZH) was synthesized, and its experimental results were compared with theoretical data. The synthesized HTM (DCZH) exhibited favourable photophysical properties and appropriate highest occupied molecular orbitals (-5.26 eV) energy levels for compatibility with perovskite materials. The photophysical characteristics of DCZH, including its Solvatochromism in various solvents and aggregation-induced emission enhancement (AIEE) behaviour in a THF: H_2O mixture, were systematically investigated. We also investigated the influence of fluoro and cyano-substituted carbazole structures on Frontiers molecular orbitals and the density of states using DFT techniques. The predicted features of the investigated HTMs indicated that these newly developed carbazole derivatives, particularly DCZH, exhibit properties consistent with efficient HTMs and therefore show potential as candidates for future application in perovskite solar cells.

1. Introduction

Perovskite solar cells (PSCs) have gained notable interest in recent years because to their extraordinary optoelectronic capabilities, resulting to a rise in power conversion efficiency (PCE) from 3% in 2009 to 26.1% in 2025 [1–3]. The facile synthesis, solution processability, and cost-effectiveness of perovskite materials make them competitive alternatives to commercially available silicon solar cells [4,5]. These unique materials possess exceptional characteristics, including a broad absorption range, high absorption coefficient, long diffusion length, and excellent charge carrier mobility, enabling efficient light-to-electricity conversion [6,7]. In PSC devices, the hole-transporting layer (HTL) plays a crucial role in extracting and transporting holes from the perovskite layer to the anode, while simultaneously blocking electron transfer [8,10]. The HTL is also vital in minimizing charge recombination and improving device stability. The 2,2′,7,7′-tetrakis(*N,N*-dimethoxyphenyl-amine)-9,9′-spirobifluorene (Spiro-OMeTAD) remains the benchmark HTM due to its high performance; however, its reliance on dopants and additives introduces issues such as instability, degradation, and increased fabrication costs, hindering the large-scale commercialization of PSCs [11,12].

Recent efforts have focused on developing dopant-free HTMs that overcome these limitations while maintaining high performance [13–15]. Various heterocyclic fused rings, such as triazatruxene,

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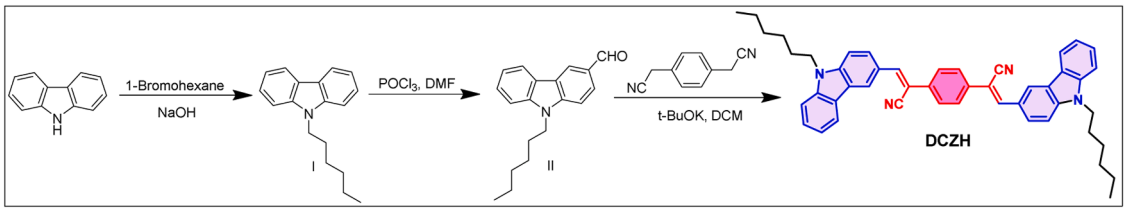

Scheme 1. Synthetic route of DCZH.

spirofluorene, cyclobenzodithiophene, carbazole, phenazine, and acridine derivatives, have been explored for this purpose. Among these, carbazole-based HTMs are promising materials due to their electron-rich nature, low redox potential, favourable optical properties, and excellent thermal and chemical stability [16–21]. For instance, Qi *et al.* designed and synthesized HTMs (CY3, CY4, CY5) based on carbazole-diphenylamine as the core, adjusting the side chain with different aromatic conjugation groups [22]. The calculated results indicated that with extension of π-conjugation showed better energy level alignment, good photophysical properties, and higher hole mobility. In PSC devices, the PCE increased from 21.28% for CY3 to 22.01% for CY5 due to a higher hole mobility, a smoother film morphology, and an effective passivation of the interface radiative recombination than CY3 and CY4. Xia *et al.* [23], developed a fused carbazole dimer end-capped with 4,4′-dimethoxy-diphenylamine (NCz-DM) as dopant-free HTMs for PSC devices. This NCz-DM exhibits a well-matched energy level, excellent hole transporting, and film formation property, results in a higher PCE of 24.0% with better device stability. Further, the incorporation of electron-withdrawing cyano (-CN) groups into electron-rich carbazole cores has proven to be a promising strategy for enhancing hole-transporting properties [24]. The cyano groups, known for their strong electron-accepting nature, increase the electron-deficient character of the molecule, thereby improving hole extraction and transport capabilities [25,26]. Cyano-containing donor-acceptor conjugated systems are widely recognized for their structural diversity, higher hole mobility, and potential as dopant-free HTMs in high-performance PSCs [27,28]. Zhou *et al.* integrated a cyano unit into the hexyl side chain of carbazole N-position utilized for HTM (H123) in PSC device. This HTM serves a dual purpose of surface passivation of perovskite and efficient hole transporting characteristics, resulting in a PCE of 18.09% and improved device stability [29]. In earlier work, we designed and synthesized a donor-acceptor-donor (D-A-D) type HTM, named TPDCN, containing a dicyanovinylene core with 4,4′-dimethoxy-triphenylamine units as the end groups [30]. The cyano group effectively enhanced intramolecular charge transfer (ICT) properties, resulting in a large Stokes shift (~134 nm), improved hydrophobicity, and better photovoltaic performance. Similarly, fluorinated materials garnered substantial interest from researchers because of the strong electronegativity, surface passivation of perovskite, and hydrophobicity nature enables the long-term device stability of PSC devices [9,31]. Building on this preliminary research, we explored the use of carbazole moieties as donors and dicyanovinylene cores as electron acceptors for integration in PSC devices.

In this work, we designed and synthesized a D-A-D type carbazole derivative (2Z,2′Z)-2,2′-(1,4-phenylene)bis(3-(9-hexyl-9*H*-carbazol-3-yl)acrylonitrile) (DCZH) for PSC application. The DCZH was synthesized via an easy and cost-effective Pd-free route using low-cost starting materials. The DCZH displayed better photophysical properties, with its HOMO energy level well-matched with perovskite ($MAPbI_3$) energy levels, enabling efficient charge extraction. The photophysical properties of DCZH, including its Solvatochromism in various solvents and aggregation-induced emission enhancement (AIEE) behaviour in a THF: H_2O mixture, were systematically investigated. Additionally, density functional theory (DFT) techniques were used to investigate the changed energy levels of carbazole chemical structures that were substituted with fluoro and cyano. Finally, these material's energy levels and other characteristics were compared to conventional HTMs to demonstrate their potential for PSC applications.

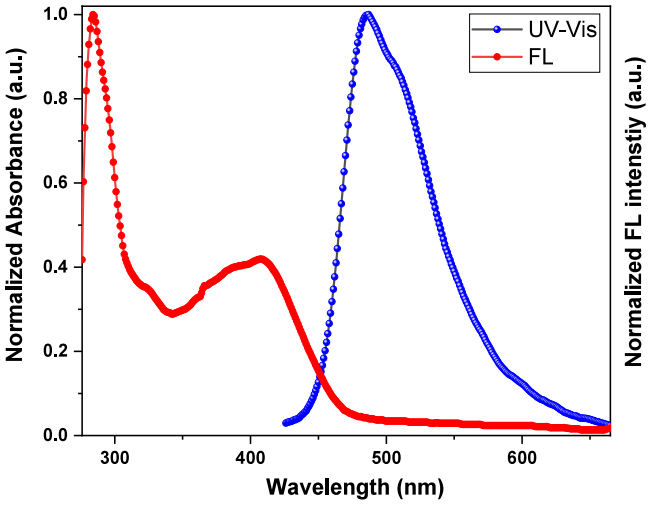

Fig. 1. UV -Visible and Fluorescence spectra of DCZH in DCM solvent.

2. Results and discussion

Scheme 1 illustrates the synthetic pathway for DCZH, and their detailed procedures are outlined in the experimental section (see supplementary material). These synthetic protocols include their concision, the employ of efficient reactions, and the use of cost-effective reagents and catalysts. Furthermore, HTM can be easily purified via simple recrystallization and column chromatography. The synthesized HTMs are examined thoroughly using FTIR, NMR, and mass spectrometry methods (Fig. S7-S9). The thermal stability of the DCZH was investigated by thermogravimetric analysis (TGA) analyses, as shown in Fig. S4. The DCZH showed a two-step degradation process: the first-step degradation T_{onset} was approximately 266 °C and was completed by 389 °C, while the second degradation step initiated at 390 °C and extended to 600 °C. The first degradation due to cleavage of aliphatic side chain and the second step degradation due to breakdown of main backbone carbazole or cyanovinylene unit [32–34]. The DCZH showed a 5% weight loss at 220 °C, excellent thermal stability of DCZH, exceeding the minimum requirements for practical integration in perovskite solar cells. The conductivity of DCZH was carried out by two probe method and obtained spectra as shown in Fig. S5. The DCZH conductivity was calculated to be 8.4×10^{-6} S/cm, which was compared with standard spiro-OMeTAD [35,36]. As we found that, our synthesized material DCZH one order higher magnitude conductive value than standard spiro-OMeTAD (10^{-7} to 10^{-6} S/cm). The synthesized materials has higher conductivity than undoped spiro-OMeTAD means the material could provide better charge extraction and less recombination loss when used as an HTM, under the same device and processing conditions.

2.6. Density of states

An examination of the density of states (DOS) provided additional support for the FMO analysis. We carried out DOS calculations, which show how different chemical orbitals contribute to electronic processes and offer insights into various energy levels, in order to confirm the FMO study. A peak at zero suggests no contribution at that energy level, but a high DOS value indicates a large contribution. The HTM molecules were divided into two fragments: the carbazole donor core at one end (Fragment 1) and the dicyanovinylene central core (Fragment 2) [59]. The DOS maps for all HTMs are presented in Fig. 9. The DOS graphs for every HTM molecule show comparable features, showing that the terminal carbazole units contribute more than the central dicyanovinylene core does for all compounds. The carbazole donor units in all HTM compounds clearly show their highest electron density distribution around the HOMO, whereas the acceptor unit shows a notable electron density spread around the LUMO. This implies that the donor and acceptor units undergo intramolecular charge transfer, which might improve the optoelectronic characteristics of PSCs [60,61].

3. Conclusion

In this study, a series of HTMs was designed to optimize their performance by introducing different electron-withdrawing units on the carbazole core and alkyl side chains. Experimental results reveal that DCZH exhibits superior photophysical properties, deep-lying HOMO energy levels compatible with perovskite, and enhanced charge extraction capability. Fluorescence results indicate that the large Stokes shifts (~90 nm) of these HTMs are beneficial for infiltration and pore-filling during PSC fabrication. Furthermore, the introduction of fluoro (-F) and cyano (-CN) groups significantly influenced the molecular configuration and energy levels of the investigated molecules. Electronic property analysis confirms that the HOMO/LUMO energy levels of these HTMs align well with the valence band and conduction band of commonly used perovskites. The predicted optoelectronic and charge transport properties suggest that these materials possess characteristics consistent with efficient HTMs and show strong potential for application in high-performance PSCs, subject to further device-level validation.

CRediT authorship contribution statement

Gayathri Kumaresan: Writing – original draft, Methodology, Investigation, Conceptualization. **Selva Kumar Ramasamy:** Writing – original draft, Methodology, Investigation, Conceptualization. **Geetha Venkatesan:** Methodology, Investigation, Conceptualization. **Ponnusamy Rohini:** Validation, Formal analysis, Data curation, Conceptualization. **Govindasamy Sathiyan:** Writing – review & editing, Writing – original draft, Supervision, Methodology, Investigation, Conceptualization.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Supplementary materials

Supplementary material associated with this article can be found, in the online version, at doi:10.1016/j.molstruc.2025.144520.

Data availability

Data will be made available on request.

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