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Proceeding Paper

Study of optical Properties of Simple carbazole in solution and as thin films Deposited via Sol-Gel Spin-Coating†

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Abstract: The elaboration and characterization of Cz-P (2,7) in solution and as thin films are the main topics of this work based on carbazole unit for perovskite solar cells. Our study focuses on studying optical properties. The elaboration of thin films was performed using sol gel spin coating onto glass substrate. Thin films deposited from different solvents were characterized by UV–vis and photoluminescence spectroscopy. The absorption maxima of investigated compounds are not significantly shifted with different solvents. The result of photoluminescence shows a green yellow emission. The optical studies reveal that the investigated material can be a promising material for the development of perovskite solar cells.

Keywords: Carbazole; hole transporting material; perovskite solar cells; Photoluminescence; thin films

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1. Introduction

Perovskite solar cells (PSCs) gained popularity after the pioneering work of Miyasaka and colleagues in the early part of 2009 [1][2]. The strength of PSCs lies in their high efficiency, which currently exceeds 25% and has the potential to surpass 30% in the future [3]. However, PSCs face several challenges that need to be overcome before they can become a widely adopted technology. One of the primary issues is their stability and durability, as perovskite materials can deteriorate in the presence of moisture or heat [4][5]. This can cause a decrease in efficiency or even the complete failure of the solar cell. To tackle this, researchers are working on developing more stable perovskite materials and encapsulation techniques to safeguard them from environmental factors. A vital component of a perovskite solar cell is the hole transport material (HTM), its primary function is to gather and facilitate the movement of positively charged carriers, commonly referred to as "holes," that are generated within the perovskite layer and transport them to the respective electrode [6]. The HTM also assumes a pivotal role in mitigating the recombination of charge carriers, a process that can adversely affect the overall efficiency of the solar cell. A frequently employed HTM is (2,2',7,7'-tetrakis(N,N-di-p-methoxyphenylamine)-9,9'-spirobifluorene) Spiro-OMeTAD, which is often doped with lithium or other additives to improve its performance [7].

Despite its popularity, there are still concerns about the stability of Spiro-OMeTAD and its relatively high cost. As a result, researchers are exploring alternative HTMs that can provide similar or better performance while addressing these issues. Carbazole-based hole transport materials (HTMs) have gained increasing attention in the field of PSCs due to its excellent hole transport properties, high thermal stability, and good solubility in common organic solvents [8][9]. These derivatives have a carbazole core with substituents at the 3, 6 or 2, 7 positions, which can modulate the energy levels and solubility of the molecules [10].

This work sought to study the effects of the solvents (Dimethylformamide, Dichloromethane, and Toluene) on the optical properties of investigated materials (as shown in Figure 1). The spin Coating method was used to prepare thin films of Cz-P(2,7). The obtained thin films were characterized by UV–vis and photoluminescence spectroscopy.

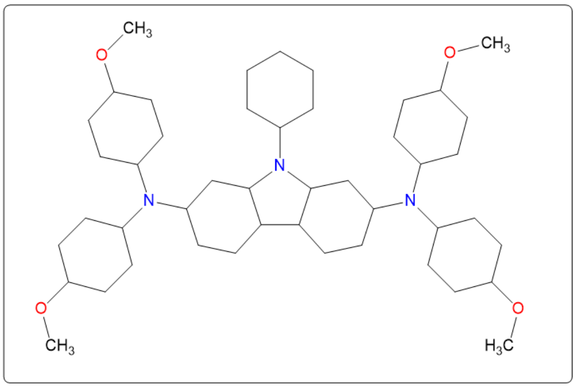

Figure 1. molecular structure of investigated material (Cz-P(2,7)).

2. Experimental methods

Prior to deposition, the glass substrate underwent ultrasonic cleaning using acetone and ethanol. The sol-gel spin coating technique was used to deposit thin films of Cz-P(2,7). The powder was procured and used without any further purification. The Cz-P(2,7) solution was prepared using toluene, dichloromethane, and chlorobenzene. The solutions were then baked at 100 °C for 30 minutes on a hot plate, resulting in a uniform brown-purple solution. At room temperature, thin films were deposited onto glass substrates that had undergone prior cleaning, using sol gel spin Coating method. UV-vis absorption measurements were taken using a PerkinElmer Lambda 2 Spectrophotometer, which operates with a double beam and can be varied in the range of 200 to 1050 nm. For photoluminescence (PL) measurements, we employed a FluoroMax-4 apparatus equipped with FluorEssence software. The excitation source utilized was a 150-W ozone-free xenon arc-lamp, while both the excitation and emission monochromators were equipped with reflection gratings boasting 1200 grooves mm^{-1}.

Photophysical properties of Cz-P(2,7) based carbazole were assessed in different solvents. All solutions were also prepared with low concentrations solution (10^{-5} M) in order to limit the aggregation effects [11]. The optical transmittance spectrum of Cz-P(2,7) was measured in different kinds of solvents from more polar to non-polar solvents. The measurements were taken for solutions as well as thin films that were deposited using spin coating at room temperature. Dimethylformamid, Dichloromethane and Toluene were selected as solvents.

3. Results and discussion

The UV-visible electronic absorption spectra of the Cz-P(2,7) depicted in Figure 2 indicate that when the polarity of the solvent increases, the absorption spectra of investigated molecule have similar trends in solution. This can be attributed to the solvents influencing the morphology of the film without altering its optical properties [12]. The absorption spectra in thin film shows a small bathochromic shift (5 nm), indicating the presence of inter-chain interactions in the solid state [13]. According to figure 2 ,Two absorption peaks are observed, first at around 300 nm attributed to the π–π* transitions

,and at lower energy absorption bands observed at >350 nm, that can be assigned as n–π* bands [14]. Cz-P (2,7) in chlorobenzene solvent presents a small band at 500 nm which may be ,corresponding to the oxidization of molecule in chlorobenzene solvent. The investigated compound shows their transparent behavior in the visible wavelength avoiding the screen effect and competition for the exciton charge separation with the perovskite layer [15].

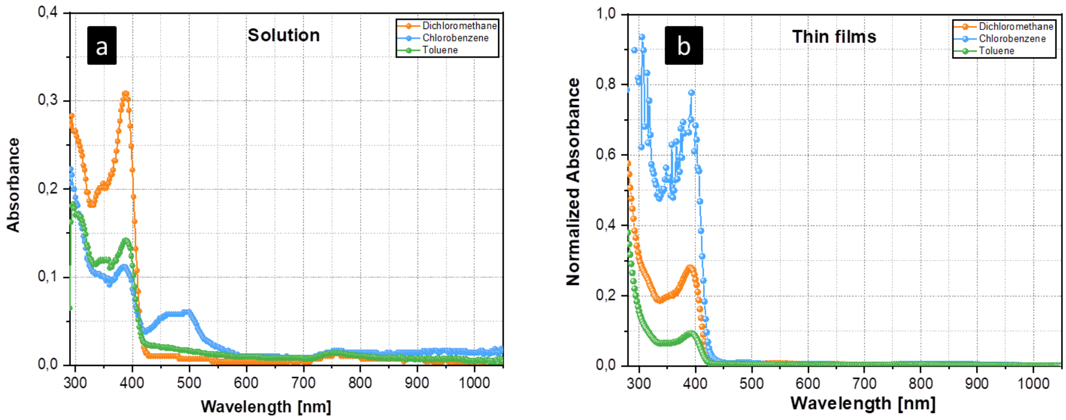

Figure 2. The absorption spectra of Cz-p (2,7) measured in Dichloromethane, chlorobenzene and Toluene Solvents.

To gain insight into the electronic structure, photoluminescence (PL) emission spectra have been recorded (Figure 3). Emission measurements were performed in dichloromethane and chlorobenzene, as a polar solvent also in Toluene as a non-polar solvent. The luminescent spectra of Cz-p (2,7) in solutions (except for dichloromethane) are also similar in features, displaying deep blue emissions at approximately 460 nm. When the polarity of the solvent is decreased, there is no drastic shift with the absorption and fluorescent emission spectra of the derivatives, indicating that the nature of the lowest singlet excited state is of π,π* transition [16]. The PL curves show a different behavior related to thin films. Similar trends were observed that's means a red-shifted absorption profile was observed in the case of comparing thin film with solutions. This red shift of emission spectra with the solvent polarity is classical for D-A systems and indicates the high polarity of the excited state (strong dipole moment) in comparison with its ground state [17].

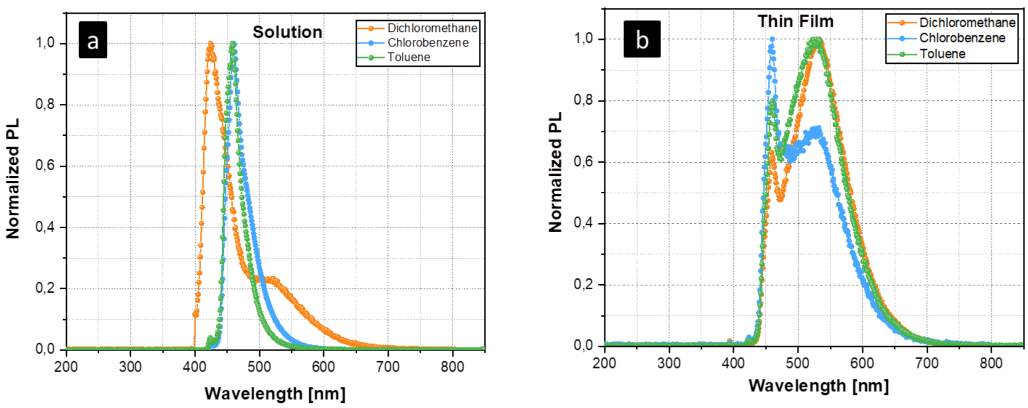

Figure 3. photoluminescence spectra of Cz-P(2,7) at room temperature measured in different solvents (Toluene, Dichloromethane, and Chlorobenzene).

3. Conclusion

The investigation of three different solutions prepared from dichloromethane, dichlorobenzene, and toluene solvents, utilized in the deposition of thin films via the sol-gel spin-coating method has been successfully done. The analysis, conducted through transmittance measurements and photoluminescence, underscores the promising qualities of these thin films. The transmittance measurements indicate a notably high level of transparency in the visible spectrum, coupled with good absorption in the UV domain. Moreover, photoluminescence measurements conducted at room temperature exhibit a distinctive green-yellow emission spectrum.

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