

Optimization of ZnPc and TPA-ZnPc phthalocyanines as hole transport materials to improve the performance of perovskite solar cells

Mustapha Ammari¹, Mohamed Jabha², Mohamed Yaakoubi¹, Samira Kharchouf³,
Abdellah Elalaoui¹, El Houssine Mabrouk²

¹ Crystalline Materials and Engineering Team, Faculty of Sciences, University Moulay Ismail of Meknes, Morocco

² Laboratory of Materials Engineering for the Environment and Natural Ressources, Faculty of Sciences and Techniques, University of Moulay Ismail of Meknès, B.P 509, Boutalamine, 52000, Errachidia, Morocco

³ Team of Innovative Materials and Mechanical Manufacturing Processes, ENSAM, University Moulay Ismail, B.P. 15290, Al Mansour, Meknes, Morocco

Corresponding authors: Mustapha Ammari (mu.ammari@edu.umi.ac.ma) and Mohamed Jabha (m.jabha@umi.ac.ma)

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Abstract

Perovskite solar cells (PSC) are a promising alternative to silicon cells, achieving a power conversion efficiency of 25.8% in ten years. Research on alternatives is necessary. Phthalocyanines, multifunctional materials, have attracted interest in improving PSCs. Used as a hole transport material (HTM), they offer an alternative to spiro-OMeTAD and PTAA due to their low cost, stability, and electronic properties.

This work optimizes zinc phthalocyanine (ZnPc) and triphenylamine zinc phthalocyanine (TPA-ZnPc) molecules using DFT (B3LYP/6-311G (d,p)) to analyze the effect of triphenylamine substitution. Adding triphenylamine modifies molecular geometry and reduces hole transport capacity. The bandgap energies are 2.178 eV (ZnPc) and 2.062 eV (TPA-ZnPc). Although both absorb in the visible range, TPA-ZnPc exhibits enhanced absorption. ZnPc demonstrates strong potential as an hole transport material with MAPbI₃.

Keywords

DFT (B3LYP/6-311G (d,p)), hole transport material (HTM), perovskite

1. Introduction

Perovskites, although known for a long time, have revolutionized the field of photovoltaics [1, 2]. First discovered in 1839 by the German mineralogist Gustav Rose, they were named after his colleague Lev Perovski [3]. Today, hybrid organic-inorganic perovskites are particu-

larly used in solar cells and optoelectronics due to their excellent semiconducting properties, including a direct bandgap, high absorption coefficient, high charge mobility, and low exciton binding energy [4].

Perovskite solar cells (PSC) represent a promising alternative, combining cost-effectiveness and efficiency comparable to traditional silicon solar cells [5]. Over the

past decade, the power conversion efficiency (PCE) of PSC devices has significantly improved, increasing from 3.8 % to 25.8% [6]. This enhancement is attributed to the properties of perovskite materials, including an adjustable bandgap, high absorption coefficient, excellent charge mobility, and extended charge carrier diffusion length [7]. Perovskite solar cells use a perovskite layer between hole and electron transport layers. The hole transport material (HTM), including several non-planar organic molecular structures such as triphenylamine and spiro-OMeTAD, are currently being studied [8–10]. However, their high synthesis costs and complex processes limit their large-scale use. Furthermore, these materials have drawbacks such as low charge mobility, reduced stability, and lower power conversion efficiency, driving research toward more efficient HTM [11, 12]. Small organic molecules offer better reproducibility due to the flexibility in structural modifications, improving their purity, mobility, and optical properties [13–15].

In recent years, phthalocyanines have emerged as a promising alternative in various fields. Phthalocyanines are commonly used in PSCs as HTMs due to their ease of preparation and purification, low synthesis cost, and thermal and chemical stability [16].

This study aims to compare the properties of unsubstituted zinc phthalocyanine (ZnPc) and substituted triphenylamine zinc phthalocyanine (TPA-ZnPc), as shown in Fig 1, which presents these two molecules. The use of density functional theory (DFT) theory has proven to be an effective method for predicting the geometry, electronic structure, and properties of conjugated materials [17]. Theoretical studies allow for the determination of key information such as the bandgap, as well as the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) levels, which are essential for the design of compounds suitable for solar cells [18].

2. Material and methods

In the present study, the ground-state geometries of the ZnPc and TPA-ZnPc molecules were optimized using DFT at the B3LYP/6-311G(d,p) level.

The electronic properties, including HOMO–LUMO energies, band gap, Mulliken atomic charges, and molecular electrostatic potential (MEP) maps, were determined from the optimized structures. Visualization and post-processing of the results were performed using GaussView 6.0 [19].

3. Results and discussion

3.1. Geometric parameters

The optimized geometries of ZnPc and TPA-ZnPc by DFT method (B3LYP/6-311G(d,p)) [20, 21] are shown in Fig. 2. Our calculations indicate that both molecules exhibit a planarity characteristic of this type of structure. Furthermore, we observed that ZnPc is more planar than TPA-ZnPc, with this change attributed to the substitution by the triphenylamine group. A more homogeneous distribution of charge across the molecule can enhance the overlap between the HOMO of the HTM and the valence band maximum of the perovskite, thereby facilitating more efficient charge extraction and limiting recombination [22].

3.2. IP, EA, and reorganization energy

Ionization potential (IP), electron affinity (EA), and reorganization energy are crucial parameters that help us understand the behavior of HTM materials [23] for efficient

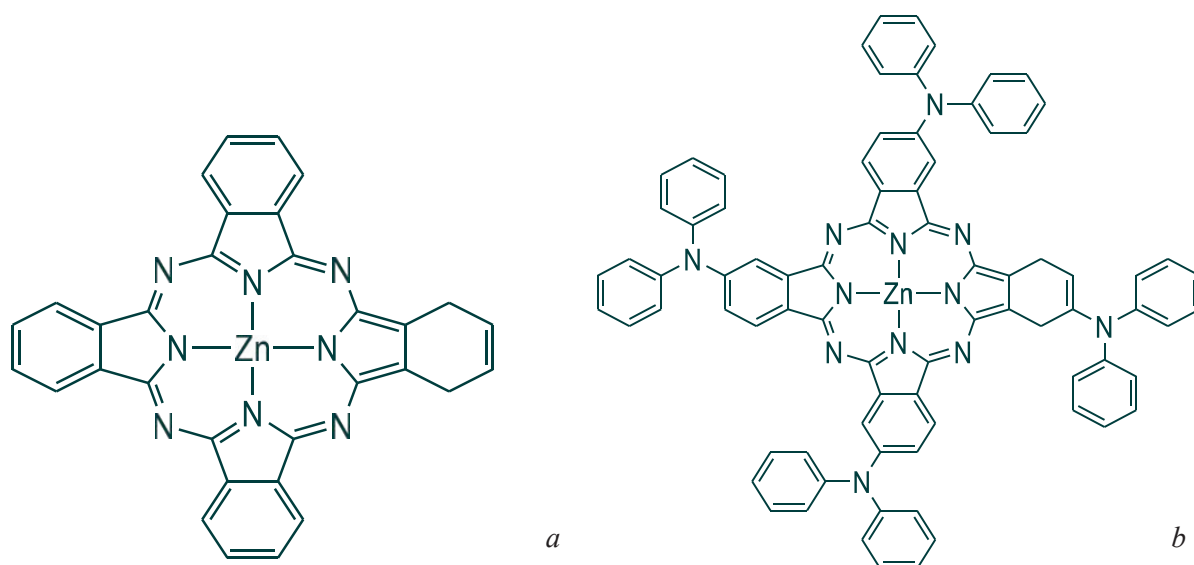


Figure 1. Molecular structure of the studied HTMs (a) ZnPc, (b) TPA-ZnPc

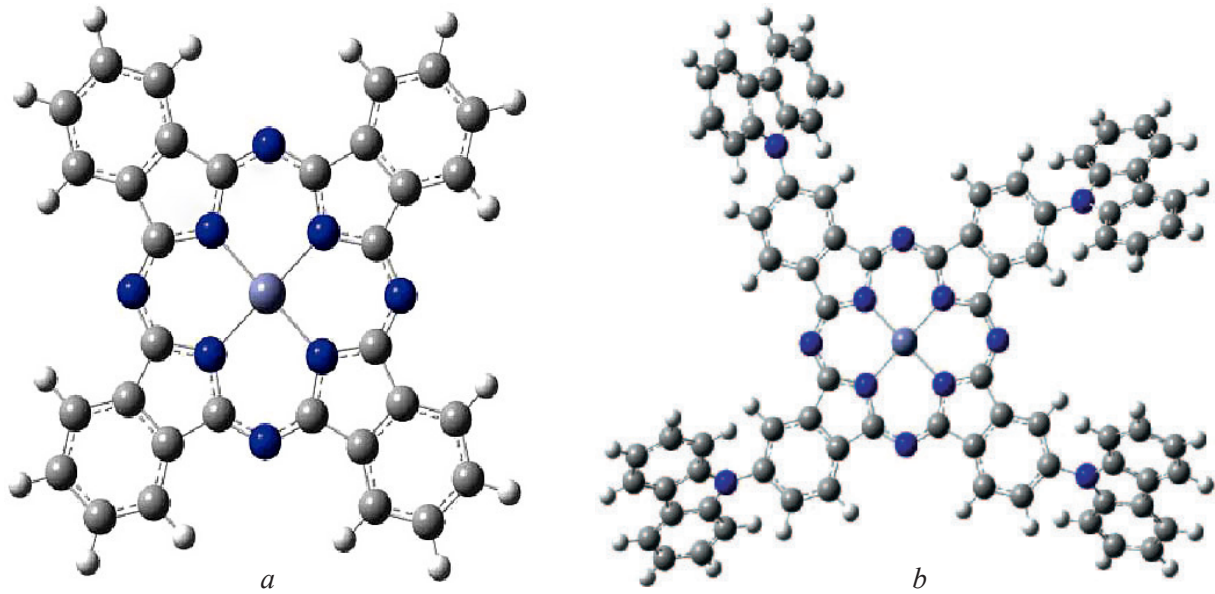


Figure 2. Optimized structures of (a) ZnPc, (b) TPA-ZnPc, obtained using the DFT/B3LYP method with the 6-311G basis set

charge transfer and optimized photovoltaic conversion in solar cells [24, 25].

During the operation of a perovskite solar cell, an electron from the HOMO of the HTM must fill the hole left in the valence band of the perovskite after the excitation of another electron [26, 27]. To facilitate this hole transfer, the IP of the HTM must be sufficiently low [26]. The lower the IP value, the easier it is to form holes in the analyzed molecules [28]. ZnPc and TPA-ZnPc have ionization energies of 6.204 eV and 6.073 eV, respectively, allowing their use as HTMs with MAPbI₃ perovskite.

Similarly, the EA indicates the ability of a material to undergo reduction. The electron affinity of the materials is 1.959 eV and 2.4 eV, respectively. These IP and EA values were obtained directly from the frontier molecular orbital energies (HOMO and LUMO) using Koopmans' theorem, as indicated in Eqs. (1) and (2).

$$IP = E_c - E_n, \quad (1)$$

$$EA = E_n - E_a. \quad (2)$$

The reorganization energy is one of the fundamental criteria to consider when designing an HTM [29]. A low reorganization energy promotes efficient charge transfer [30]. The total reorganization energy (λ_{total}) corresponds to the sum of the reorganization energies of the electrons (λ_e) and holes (λ_h) [31]. It is defined by the following expression:

$$\lambda_e = (E_n^- - E_a) + (E_n^0 - E_n); \quad (3)$$

$$\lambda_h = (E_n^+ - E_c) + (E_c - E_n); \quad (4)$$

$$\lambda_{\text{total}} = \lambda_e + \lambda_h, \quad (5)$$

where E_c , E_a , and E_n correspond to the total energies of the cation, anion, and neutral system in their optimized geometries, respectively. E_n^+ and E_n^- represent the en-

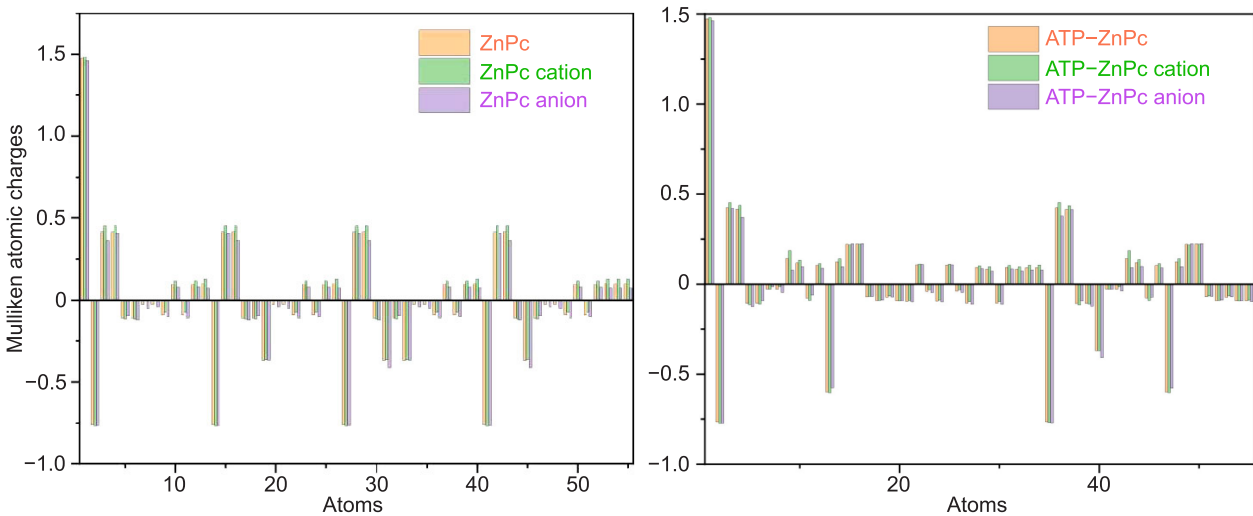


Figure 3. Graph of Mulliken atomic charges

Table 1. Reorganization energies (λ), charge transfer integral (V), charge transfer rate (K), global electrochemical potential (μ), and hardness (η) for ZnPc and TPA-ZnPc

Molecules	λ_h (eV)	λ_e (eV)	λ_{total} (eV)	V_h (eV)	K_h (s ⁻¹)	V_e (eV)	K_e (s ⁻¹)	μ (eV)	η (eV)
ZnPc	0.195	0.143	0.338	1.91	$3.55 \cdot 10^{15}$	-1.087	$3.99 \cdot 10^7$	4.08	2.12
TPA-ZnPc	0.544	0.330	0.874	0.27	$1.17 \cdot 10^{12}$	0.0464	$4.09 \cdot 10^{13}$	4.23	1.83

ergies of the cationic and anionic systems, calculated at the optimized geometry of the neutral state. Finally, E_c^0 and E_a^0 denote the energies of the neutral system evaluated at the optimized geometries of the cation and anion, respectively [32].

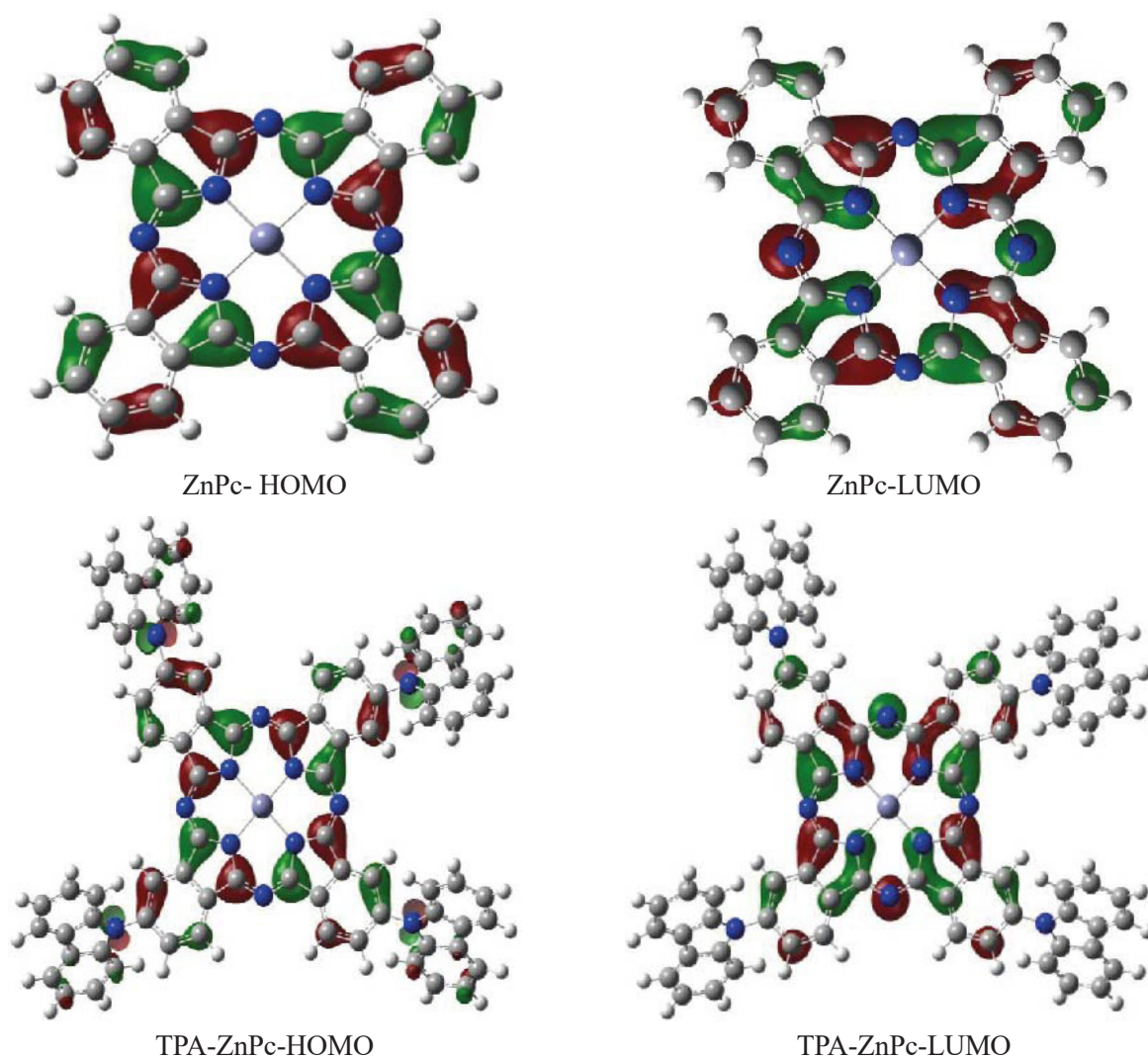
3.3. Mulliken charge

HTM materials are responsible for transporting holes (positive charge), so the study of Mulliken charges of the cation is particularly essential [33]. The charges represent in Fig. 3. The positive charges for ZnPc and TPA-ZnPc are well distributed, indicating that the molecule will

have good hole mobility, which is crucial for applications in solar cells. The x-axis represents the atoms numbered according to their order in the Gaussian output file. The value “0” corresponds to the reference level of atomic charge used for comparison, and numbering starts from the central Zn atom and proceeds clockwise along the macrocycle.

3.4. Charge transfer rate (K)

Marcus theory is used to confirm the nature of charge transfer, as studying the reorganization energy alone is not sufficient [13]. According to the calculation of the

**Figure 4.** Representations of the HOMO and LUMO surfaces of ZnPc and TPA-ZnPc in the gas phase, obtained using the DFT/B3LYP method with the 6-311G basis set

hole and electron transfer rates of ZnPc and TPA-ZnPc using Eqs. (6) and (7), it is observed that ZnPc has a faster hole transfer rate compared to TPA-ZnPc, but a lower electron transfer rate.

$$k_h = \frac{V^2}{h} \left(\frac{\pi}{\lambda_h k_B T} \right)^{1/2} \exp \left(\frac{\lambda_h}{4k_B T} \right); \quad (6)$$

$$k_e = \frac{V^2}{h} \left(\frac{\pi}{\lambda_e k_B T} \right)^{1/2} \exp \left(\frac{\lambda_e}{4k_B T} \right); \quad (7)$$

where V represents the charge transfer integral, λ corresponds to the reorganization energy, k_B is the Boltzmann constant, and T is the temperature, typically set to 300 K. Based on the equation above, the hole hopping rate (k_h) primarily depends on two key parameters: V and λ . These parameters are actually divided into two simple components: the electron transfer integral (V_e) and the hole transfer integral (V_h) [34]. These are calculated respectively using the following equations [35]:

$$V_h = (E_{\text{HOMO}} - E_{\text{HOMO}-1})/2, \quad (8)$$

$$V_e = (E_{\text{LUMO}} - E_{\text{LUMO}+1})/2. \quad (9)$$

3.5. Global electrochemical potential (μ) and hardness (η)

Calculations of the chemical potential and hardness confirm the chemical stability of the studied compounds [36]. Equations (10) and (11) were used to calculate the chemical potential (μ) and hardness (η). The results, presented in Table 1, show that ZnPc has a lower electrochemical

potential than TPA-ZnPc, indicating greater electrochemical stability.

$$\mu = (\text{IP} + \text{EA})/2; \quad (10)$$

$$\eta = (\text{IP} - \text{EA})/2. \quad (11)$$

3.6. Frontier molecular orbitals (HOMO–LUMO)

The distribution of the HOMO and LUMO of the studied HTM molecules is shown in Fig 4 below. This representation provides a general understanding of the electronic structure [25]. From these results, we can say that both HTM molecules exhibit good charge transport properties. It is observed that the electronic density of the HOMO and LUMO orbitals extends over the entire molecule.

3.7. Bandgap energy

Table 2 presents the results obtained for the HOMO, LUMO, and E_g energies of the two molecules, ZnPc and TPA-ZnPc. For a molecule to be designed as an HTM, the HOMO must be lower than the maximum valence band level of the perovskite to promote hole extraction and minimize energy losses at the interfaces [37]. Additionally, the LUMO must be sufficiently high to block

Table 2. Energies of the HOMO, LUMO molecular orbitals and the energy gap (in eV) for ZnPc and TPA-ZnPc

Molecules	E_{HOMO} (eV)	E_{LUMO} (eV)	E_g (eV)
ZnPc	−5.1609	−2.9829	2.1780
TPA-ZnPc	−5.3811	−3.3190	2.0621

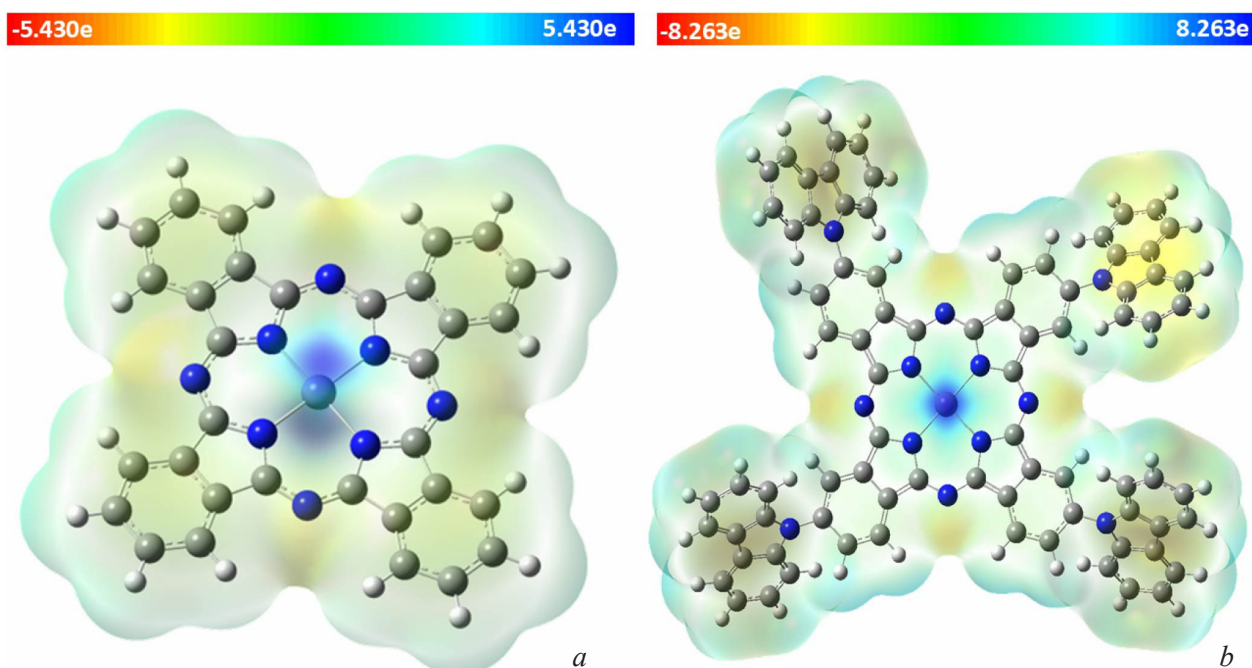
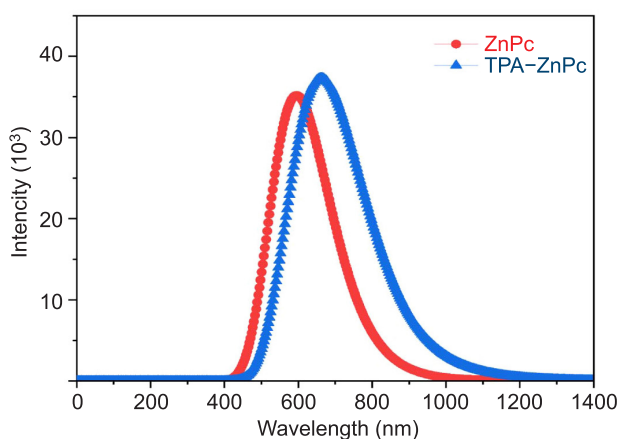


Figure 5. Electrostatic potential (MEP) surfaces of (a) ZnPc and (b) TPA-ZnPc

Table 3. Maximum absorption wavelength ($\lambda_{\max}$) of ZnPc and TPA-ZnPc in the gas phase

Molecules	E_{ex} (eV)	$\lambda_{\max}$ (nm)	F_{osc}	Types of excitations	% of distributions
ZnPc	2.0818	595.56	0.4343	H-4 $\rightarrow$ L+1	-17.098
				H $\rightarrow$ L	68.777
	2.0820	595.52	0.4341	H-4 $\rightarrow$ L	17.103
				H $\rightarrow$ L+1	68.774
	3.1945	388.12	0	H-5 $\rightarrow$ L	70.561
TPA-ZnPc	1.8670	664.09	0.4654	H-4 $\rightarrow$ L+1	15.179
				H-1 $\rightarrow$ L	10.283
				H $\rightarrow$ L+1	66.828
	1.8714	662.53	0.4400	H-4 $\rightarrow$ L	16.258
				H $\rightarrow$ L	67.339
	2.0529	603.95	0.0202	H-3 $\rightarrow$ L	27.438
				H-2 $\rightarrow$ L	14.072
				H-2 $\rightarrow$ L+1	33.535

**Figure 6.** Absorption spectra of ZnPc and TPA-ZnPc

electrons and thus reduce charge recombination [38, 39]. ZnPc and TPA-ZnPc have respective bandgap energies of 2.178 eV and 2.062 eV. We observed a decrease in the bandgap energy following the addition of the triphenylamine group. This reduction is due to the increase in the energy of the HOMO.

3.8. Molecular electrostatic potential

To analyze the electronic density and possible hydrogen bonds with the HTM material, it is necessary to estimate the MEP (Fig. 5) through a calculation based on the DFT/B3LYP/6-311(d,p) method [41].

Based on this representation, and using the electrostatic potential values illustrated by a colored diagram, we observed that there are no negative values or red regions, indicating the absence of potentially electrophilic sites [41, 42]. On the other hand, a region with a positive charge, indicated in blue, is observed around the nitrogen atom.

3.9. Absorption Spectra

We obtained the absorption properties using the TD-DFT technique with a 6-311G basis set on the optimized gas-phase structures (Fig. 6). Additionally, we calculated the maximum absorption wavelengths ($\lambda_{\max}$) and identified the electronic transitions. All of these results are presented in Table 3. We observe that both ZnPc and TPA-ZnPc exhibit absorption wavelengths in the visible region. The absorption peak intensities of TPA-ZnPc in the visible range are higher than those of ZnPc. This increase may be due to the new electronic transitions induced by the TPA group. Furthermore, we observe a shift in the TPA-ZnPc spectrum. This difference is attributed to the presence of the triphenylamine group as a substitution.

Conclusions

To analyze the impact of the substitution of ZnPc by triphenylamine (TPA) on its structural and electronic properties, we used the DFT method (B3LYP/6-311G (d,p)). The addition of the TPA group modifies the geometry of the molecule and reduces its hole-transport capacity. The analysis of the ionization potential (IP) shows that ZnPc and TPA-ZnPc have values of 6.204 eV and 6.073 eV, respectively, promoting their role as hole transport materials (HTMs). Moreover, the calculations of the chemical potential and hardness confirm the chemical stability of the studied compounds. The electrochemical potential results indicate that ZnPc possesses better electrochemical stability than TPA-ZnPc.

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Author contributions

Conceptualization: Mustapha Ammari, Mohamed Jabha; Methodology: Mustapha Ammari, Mohamed Jabha, Mohamed Yaakoubi; Writing – preparation of the original

draft: Mustapha Ammari, Writing – revision and editing: Samira Kharchouf, El Houssine Mabrouk; Supervision: Abdellah Elalaoui, El Houssine Mabrouk; Administration of the project: Abdellah Elalaoui; All the authors have read and accepted to the published version of the manuscript.

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