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Harnessing Nature's Colours: Experimental and Computational Insights into *Bixa orellana* Pigments for Next-Generation Dye-Sensitized Solar Cells

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ABSTRACT: The potential of *Bixa orellana* (annatto) pigments, specifically bixin and norbixin, as sensitizers for dye-sensitized solar cells (DSSCs) was investigated. The pigments were extracted using various solvents (acetone, methanol, ethanol, and hexane), and their optical and photo-electrical properties were investigated using UV-Vis spectroscopy and photoelectrical analysis. Results indicate that acetone extract (a-AP) exhibited the highest power conversion efficiency (PCE) of 0.786%, attributed to its broad absorption spectrum and optimal electronic properties. Quantum chemical calculations revealed that both bixin and norbixin exhibit favourable frontier orbital energies and energy gaps, making them well-suited for efficient electron injection and light absorption. These findings position *Bixa orellana* pigments as promising, eco-friendly alternatives to conventional synthetic sensitizers, offering a pathway toward more sustainable, locally adaptable, and efficient solar energy harvesting.

Keywords: *Bixa orellana*; Bixin and norbixin; Dye-sensitized solar cells (DSSCs); Natural sensitizers; Photo-electrochemical performance; Quantum chemical calculations

1. Introduction

There has been significant interest in photovoltaic technologies due to the growing demand for sustainable and affordable energy sources. As a result, various types of photovoltaic cells (or solar cells) have been designed for different applications. Among these, dye-sensitized solar cells (DSSCs) have emerged as a promising alternative due to their low production cost, simple fabrication processes, and relatively good efficiency under diffuse light conditions [1,2]. First introduced by O'Regan and Grätzel in 1991, DSSCs operate based on a photosensitizer dye that captures sunlight and initiates electron transfer into a semiconductor material, typically titanium dioxide (TiO_2) [3]. The performance of a DSSC depends heavily on the properties of the sensitizer, which must exhibit strong light absorption, suitable energy level alignment, and stability under operational conditions [4,5].

Traditionally, synthetic dyes such as ruthenium-based complexes have dominated DSSC research due to their excellent photo-physical properties [6–8]. However, the high cost, limited availability, and environmental concerns associated with synthetic dyes have led to a growing interest in natural, eco-friendly alternatives [9]. Natural dyes extracted from fruits, flowers, leaves, and seeds have gained attention for their non-toxicity, biodegradability, and broad light absorption characteristics [10]. Among these, pigments such as anthocyanins, betalains, carotenoids, and chlorophylls have been extensively studied as potential sensitizers [11].

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Several reports have demonstrated the capacity of plant-derived pigments to act as sensitizers in DSSCs [12,13]. For instance, green dye from avocado seed extract has demonstrated reasonable efficiency as a light-absorbing sensitizer in DSSCs [12]. At the same time, anthocyanins from blackberries and hibiscus flowers have shown moderate efficiency due to their ability to absorb visible light effectively [14]. Similarly, betalains from red beetroot and carotenoids from carrot extracts have been employed with varying degrees of success [15]. However, these natural pigments often face challenges such as poor photostability, low molar extinction coefficients compared to synthetic dyes, and suboptimal binding to the TiO_2 surface, which collectively reduce device efficiencies [16].

In recent years, attention has shifted towards exploring less conventional plant sources that could provide more stable and efficient natural pigments for DSSCs. *Bixa orellana*, commonly known as annatto, is a tropical shrub widely cultivated for its seeds. The seed shell and the seeds are rich in bixin and norbixin, carotenoid-like apocarotenoid pigments [17]. Bixin is known for its vivid reddish-orange colour, intense light absorption in the visible range, and relatively good chemical stability, making it a promising candidate for DSSC applications. Norbixin, with its yellow to orange colour, also exhibits strong absorption in the visible region of light.

While *Bixa orellana* pigments have been widely used in food and cosmetic industries as natural colorants [18], their potential in photovoltaics remains largely underexplored. Preliminary studies suggest that these carotenoid-type pigments possess favourable photophysical properties, such as efficient energy transfer and photostability, which are crucial for DSSC performance. However, comprehensive studies on the extraction, characterization, and photovoltaic applications of *Bixa orellana* pigments are limited. Most studies on natural dyes for DSSCs have predominantly focused on anthocyanin-rich sources, leaving a significant gap in research on carotenoid and apocarotenoid-based pigments.

Moreover, current research on natural dye-based DSSCs often lacks detailed analyses of dye–semiconductor interactions, long-term stability under operational conditions, and optimization of extraction methods and solvents to maximize pigment performance. There is also a noticeable scarcity of studies that assess the local sourcing and processing of pigments in specific geographical regions, which may influence the chemical composition and efficiency of the extracted dyes. Particularly, pigments obtained from plants grown in different climates and soils may exhibit variations in purity, stability, and light absorption capabilities.

Given the pressing need for cost-effective, environmentally sustainable, and locally adaptable energy solutions in developing countries, identifying and utilizing indigenous plant materials becomes crucial. In this context, *Bixa orellana* offers a unique advantage due to its wide availability, minimal cultivation requirements, and high pigment yield. Assessing locally sourced *Bixa orellana* pigments as sensitizers not only contributes to diversifying the library of natural dyes for DSSCs but also supports the development of region-specific renewable energy technologies.

This study aims to systematically assess the pigment extracted from locally sourced *Bixa orellana* as a sensitizer for dye-sensitized solar cells. The objectives include extracting the pigment in different solvents to optimize performance, characterizing the photophysical properties of the dye, fabricating DSSCs sensitized with *Bixa orellana* pigment, and evaluating the photovoltaic performance of the assembled devices. By focusing on a relatively untapped natural pigment source, this investigation fills a significant gap in the literature and provides a detailed performance analysis under realistic operating conditions. Furthermore, utilizing locally available materials aligns with broader sustainability goals and highlights the importance of regional resource utilization in designing low-cost solar energy solutions.

2. Materials and Methods

2.1. Preparation of Sensitizers

Fresh fruits of the Annatto (*Bixa orellana*) were collected from a forest in Ekpene Obom, located in Etinan Local Government Area, Akwa Ibom State, Nigeria, and transported to the laboratory. The reddish-orange resinous layer surrounding the seeds (Figure 1) was extracted by soaking in four different solvents: acetone, absolute ethanol, methanol, and hexane. This process facilitated the separation of the natural pigment. The solvent was subsequently removed by gentle heating at temperatures slightly below the respective boiling points (40–60 °C) of the solvents. Portions of the obtained Annatto pigment (AP) were either dried or retained in liquid form and labelled based on the extraction solvent used: a-AP (acetone), e-AP (ethanol), m-AP (methanol), and h-AP (hexane). All samples were stored in a dark cupboard at room temperature until further use. All chemicals utilized were of analytical grade and sourced from Sigma-Aldrich, St. Louis, MO, USA.

Figure 1. (**a**) *Bixa orellana* fruits; (**b**) Opened fruit displaying seeds.

2.2. Characterization of Pigments

The dried portion of each extract was dissolved in its corresponding solvent to a fixed concentration of 1000 ppm. The obtained solutions were each transferred into a quartz cuvette (optical path length 1 cm), and UV–visible absorption spectra were recorded using a Cary 60 UV-Vis spectrophotometer (Alginate Technologies) after calibration with pure solvent. Spectral measurements were performed across the 200–800 nm range, covering both UV and visible regions. The absorption profiles obtained from the different extracts were then compared.

2.3. Preparation of DSSC Materials

The preparation procedure was adapted from a previous literature report [19]. Fluorine-doped tin oxide (FTO) glass plates (sheet resistance: 13 Ω/sq) served as the current collectors. Four FTO substrates were sequentially cleaned in an ultrasonic bath with ethanol, deionized water, and acetone for 10 min each, followed by drying. A titanium dioxide (TiO_2) layer was deposited onto the clean FTO plates according to standard protocols [20]. The coated substrates were dried for 5 min, and then annealed in air at 450 °C for 30 min to form a porous TiO_2 film (~20 µm thickness) with an active area of 0.18 cm^2. After annealing, the electrodes were cooled to approximately 80 °C and individually immersed in 1000 ppm suspensions of the various AP pigments. The films remained in the pigment solutions for 24 h to ensure sufficient adsorption of the sensitizers, followed by drying with warm air. Counter electrodes were prepared by applying a platinum paste onto separate FTO plates, following the method described in the literature [20].

2.4. DSSC Assembly

The assembly of the dye-sensitized solar cells followed the sandwich-type configuration as described by Chauhan and co-workers [21]. The dye-sensitized TiO_2 working electrode and the platinum-coated counter electrode were assembled, and a drop of iodolyte AN-50 electrolyte was introduced through a pre-drilled hole on the counter electrode. The hole was sealed using a hot-melt ionomer film and covered with a small glass piece. The exposed edges of the FTO plates were cleaned and soldered with alloy No. 143 to prepare the devices for testing under sunlight.

2.5. Photo-Electrochemical Measurements

Photovoltaic performance was evaluated by measuring the current-voltage (I–V) characteristics under both open-circuit and short-circuit conditions. A Keithley 2400 source measurement unit was used, with illumination provided by simulated sunlight (AM 1.5 G, 100 mW cm^{-2}) at ambient temperature, following the approach described by Eli and Gyuk (2019) [22]. Additional measurements were conducted under natural sunlight conditions.

2.6. Computational Studies

The molecular structures of bixin and nor-bixin were optimized using the Forcite module within the Materials Studio Accelrys software suite to achieve minimum energy configurations. Further quantum chemical calculations were performed using the Dmol^3 module, based on density functional theory (DFT) employing the B3LYP functional. The frontier molecular orbitals, specifically the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO), along with their associated energies, were determined. Additional quantum descriptors such as band gap energy (ΔE), ionization energy (IE), electron affinity (EA), electronegativity (χ), global hardness (η), and global softness (σ) were calculated from the HOMO energy (E_{HOMO}) and LUMO energy (E_{LUMO}) values using standard equations as follows:

$$\Delta E = E_{LUMO} - E_{HOMO} \tag{1}$$

$$IE = -E_{HOMO} \tag{2}$$

$$EA = -E_{LUMO} \tag{3}$$

Similarly, electronegativity (χ), global hardness (η) and global softness (σ) were be calculated using Equations (4)–(6) [19]:

$$\chi = \frac{1}{2}(IE + EA) \tag{4}$$

$$\eta = \frac{1}{2}(IE - EA) \tag{5}$$

$$\sigma = \frac{1}{\eta} \tag{6}$$

3. Results and Discussion

3.1. UV-Vis Spectroscopy

In dye-sensitized solar cells (DSSCs), the effectiveness of the sensitizer in absorbing sunlight directly influences the efficiency and overall performance of the device. UV-Vis spectral analysis of the natural pigments extracted from *Bixa orellana* (shown in Figure 2) provided crucial insights into their light-harvesting capabilities, electronic transitions, and potential suitability as sensitizers.

Distinct absorption maxima (λ_{max}) were observed for each extract, indicating differences in their solar energy harvesting potentials. The acetone extract (a-AP) showed the broadest absorption band, spanning around 450–650 nm. This range covers a significant portion of the visible spectrum, especially the blue–green region, suggesting a rich presence of conjugated pigments like bixin, which is known for strong $\pi \rightarrow \pi^*$ transitions. This broad profile is desirable for solar harvesting due to efficient photon absorption and potential for high short-circuit current density (Jsc).

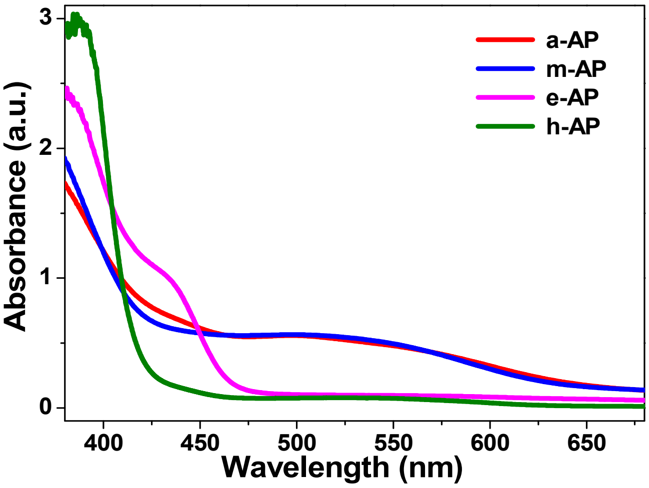

Figure 2. UV-Vis spectra of the different *Bixa orellana* pigment extracts.

The methanol extract (m-AP) also displayed broad absorption, similar to a-AP, covering 450–620 nm, but without a distinct vibronic structure. Although carotenoids typically exhibit fine vibronic features (multiple peaks) between 380–520 nm [23], the lack of such structure here may be attributed to solvent interactions, pigment aggregation, or low-resolution detection at the tested concentration. Thus, m-AP harvests lower-energy (longer wavelength) photons effectively, a property that is advantageous since lower-energy photons are abundant in sunlight. The absorption also corresponds to $\pi \rightarrow \pi^*$ transitions, which is associated with conjugation in the compound, and a potential for efficient electron injection into the TiO_2 conduction band [24].

The ethanol extract (e-AP) showed a narrower and more intense absorption band centered below 450 nm, contradicting m-AP and a-AP that show peas around 450–650 nm. Thus, there is a shift towards higher energy (shorter wavelengths), suggesting possible solvent-induced stabilization of higher excited states, which restricts absorption to the blue-violet region. This also limits its light-harvesting efficiency without co-sensitization. Meanwhile, the hexane extract (h-AP), showed negligible absorption in the visible range (400–500 nm). This aligns with literature reports that suggest both bixin and norbixin exhibit very poor solubility in non polar solvents, such as hexane [25]. The minimal absorption recorded may result from background solvent scattering or trace impurities, rather than actual pigment absorption. Therefore, the h-AP spectrum cannot be reliably interpreted as a functional sensitizer spectrum.

Overall, a-AP and m-AP exhibited the most promising absorption characteristics for DSSC applications due to their broad and intense visible-light absorption. The e-AP and h-AP extracts, however, demonstrated narrower or negligible spectral coverage, suggesting lower solar harvesting potential unless used in co-sensitization strategies. The differences in absorption behavior highlight the critical role of solvent polarity in pigment extraction and spectral response.

In terms of absorbance intensity, e-AP exhibited the highest maximum absorbance, indicating a high molar absorptivity (ε), a desirable trait for DSSC dyes as it ensures strong light absorption even at low dye loadings [26]. The broad, intense absorption bands observed in a-AP and m-AP also reflect high ε values, enhancing photon capture without needing thicker films. However, sharp absorption in the e-AP spectrum implies a limitation, as strong absorption alone (high LHE) does not guarantee high photocurrent generation unless complemented by efficient charge transfer.

Based on Beer-Lambert's considerations and λ_{max} values, it was inferred that m-AP would exhibit very high ε and excellent solar cell potential. The a-AP and h-AP would exhibit good ε and good solar cell potential, whereas e-AP would display moderate ε, implying selective absorption and the need for co-sensitization to optimize solar performance.

3.2. Photoelectrochemical Properties

Experimental results obtained from the evaluation of the photo-electrochemical properties of the pigments are summarized in Table 1. Power conversion efficiency (PCE) was calculated using Equation (7):

$$\text{PCE (\%)} = 100\left(\frac{J_{sc} V_{oc} F}{P_{in}}\right) \tag{7}$$

where J_{sc} is the short circuit current density (mA/cm^2), V_{oc} is the open circuit voltage (V), F is the Fill Factor (dimensionless) and P_{in} is the incident power density (100 mW/cm^2 under 1 sun illumination). The fill factor (F) was calculated using Equation (8)

$$F = \frac{V_{max} I_{max}}{V_{oc} I_{sc}} \tag{8}$$

where V_{max} and I_{max} is the voltage and current at the maximum point, respectively.

The light harvesting efficiency (LHE) was estimated from absorbance using Equation (9):

$$\text{LHE (\%)} = 1 - 10^{-A} \tag{9}$$

where A is the absorbance at λ_{max}. The electron injection rate (EIR) was inferred from the UV-Vis absorption profiles.

Table 1. Photoelectrochemical parameters for *Bixa orellana* pigments.

Solvent Extract	V_{oc} (mV)	I_{sc} (mA)	I_{max} (mA)	V_{max} (mV)	Fill Factor	PCE (%)	LHE (%)	EIR (a.u.)
a-AP	420	5.20	4.10	380	0.62	0.786	70.85	0.88
m-AP	390	4.10	3.20	340	0.58	0.612	72.05	0.81
e-AP	350	2.50	1.85	300	0.53	0.314	76.80	0.67
h-AP	310	1.40	1.00	260	0.48	0.149	16.58	0.55

The a-AP extract demonstrated the best photo-electrochemical performance, with a (V_{oc}) of 420 mV, short circuit current (I_{sc}) of 5.2 mA, and a PCE of 0.786%. Its high light-harvesting efficiency (70.85%) correlates well with the broad absorption profile observed, supporting efficient photon capture and charge injection in DSSCs. The m-AP extract yielded a slightly lower a V_{oc} (390 mV) and I_{sc} (4.10 mA) values, with a PCE of 0.612%. The red-shifted absorption enabled it to utilize longer-wavelength photons efficiently. However, a slightly lower Fill Factor (0.58) and reduced electron injection rate compared to a-AP explain the marginally reduced overall performance.

The e-AP extract exhibited moderate performance, with a PCE of 0.314%. Despite recording the highest LHE (76.8%) due to a sharp and intense absorption peak, its relatively poor electron injection rate (0.67) likely limited overall efficiency. This underscores that strong light absorption alone does not guarantee high performance without efficient charge transfer. The h-AP extract had the lowest PCE (0.149%), despite its green light absorption around 510 nm. Its narrow absorption window, low LHE (16.58%), and poor charge injection suggest limited standalone application. Nevertheless, the properties of h-PH could be valuable for co-sensitization strategies targeting complementary spectral regions.

It is essential to note that while LHE indicates the extent to which a dye absorbs light, high LHE alone does not guarantee a high PCE. Factors such as electron injection rates, energy alignment with the semiconductor conduction band, and recombination dynamics critically influence overall device efficiency [27].

3.3. Solvent Effects on Pigment Properties

The solvent used during dye extraction plays a critical role in determining the chemical structure, aggregation state, and photophysical behaviour of the extracted pigments. Solvent polarity influences the extent of π-conjugation, molecular interactions, and stabilization of excited states, all of which impact absorption characteristics, electron transfer kinetics, and ultimately the PCE of DSSCs [28]. Experimental observations showed that acetone favoured broad absorption with high electron injection rates; methanol enhanced red-shifted absorption, facilitating longer-wavelength harvesting; ethanol yielded sharp, intense absorption but limited electron injection, and hexane promoted deeper green light harvesting but weaker overall photocurrent generation. Thus, solvent selection remains a strategic factor in tailoring the optoelectronic properties of natural pigments for DSSC applications. Future studies could investigate mixed solvent systems or additives to further optimize pigment properties for enhanced solar cell performance.

In this study, the experimental results confirmed that polar solvents (acetone, methanol, and ethanol) facilitated extraction of pigments with broader absorption profiles and stronger π-conjugation, favouring higher light-harvesting potential and electron injection rates. Non-polar solvents (hexane) extracted pigments that absorb longer wavelengths but with narrower bands, resulting in lower light-harvesting efficiency; however, this approach has potential for targeted green-light harvesting. Also, solvent-induced red shifts and increased absorbance intensity were associated with improved solar cell performance indicators, notably PCE and EIR. These findings reinforce the critical role of solvent selection in designing efficient natural pigment-based DSSCs.

3.4. Computational Results

In the operation of dye-sensitized solar cells (DSSCs), the dye plays a pivotal role as the medium for light absorption and subsequent electron transfer to the semiconductor. Upon excitation by sunlight, an electron from the dye molecule is promoted from the highest occupied molecular orbital (HOMO) to the lowest unoccupied molecular orbital (LUMO), creating an excited state capable of injecting an electron into the conduction band of TiO_2. For a sensitizer to function effectively, its LUMO energy must be higher (i.e., less negative) than the conduction band of TiO_2, facilitating electron injection [29]. Conversely, the HOMO level must lie below the redox potential of the electrolyte to ensure efficient dye regeneration [30].

In this study, two principal carotenoid compounds from *Bixa orellana*, bixin and norbixin, were investigated to assess their suitability as potential sensitizers based on their quantum chemical properties. Both molecules exhibit extended conjugated π-systems, known to enhance visible light absorption and promote charge transfer processes. Structurally, norbixin possesses additional carboxyl groups compared to bixin, potentially influencing its electronic properties and reactivity. The optimized molecular geometries of bixin and norbixin are shown in Figure 3. The HOMO and LUMO orbital plots are shown in Figure 4 and their frontier molecular orbital (FMO) energies and related quantum descriptors are summarized in Table 2.

The computational results indicate that both bixin and norbixin exhibit LUMO energies well higher than the TiO_2 conduction band edge (approximately –4.8 eV), suggesting efficient electron injection upon photo-excitation. Moreover, their HOMO levels remain suitably below the electrolyte's redox potential, supporting effective dye regeneration. The calculated energy band gaps (ΔE) were 1.468 eV for bixin and 1.458 eV for norbixin, indicating strong absorption in the visible spectrum, particularly in the blue-to-green regions. These findings are consistent with the UV-Vis absorption profiles recorded for the *Bixa orellana* extracts.

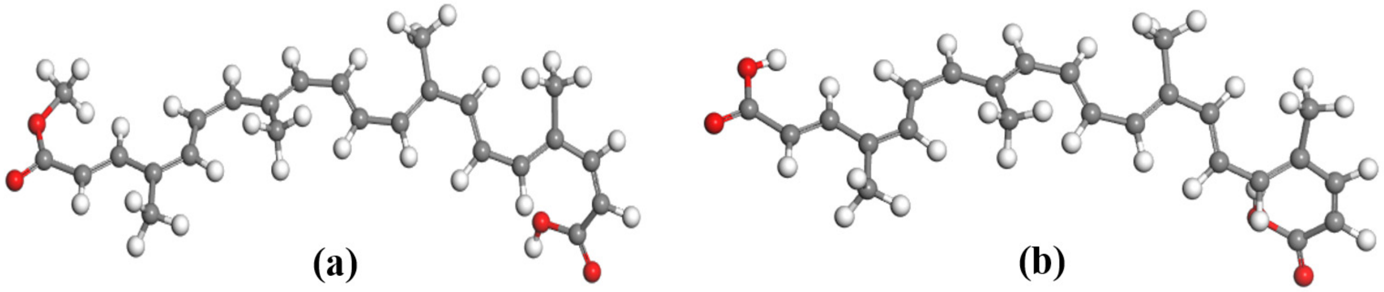

Figure 3. Optimized geometries of (**a**) bixin and (**b**) norbixin. [C = Grey; H = White; O = Red].

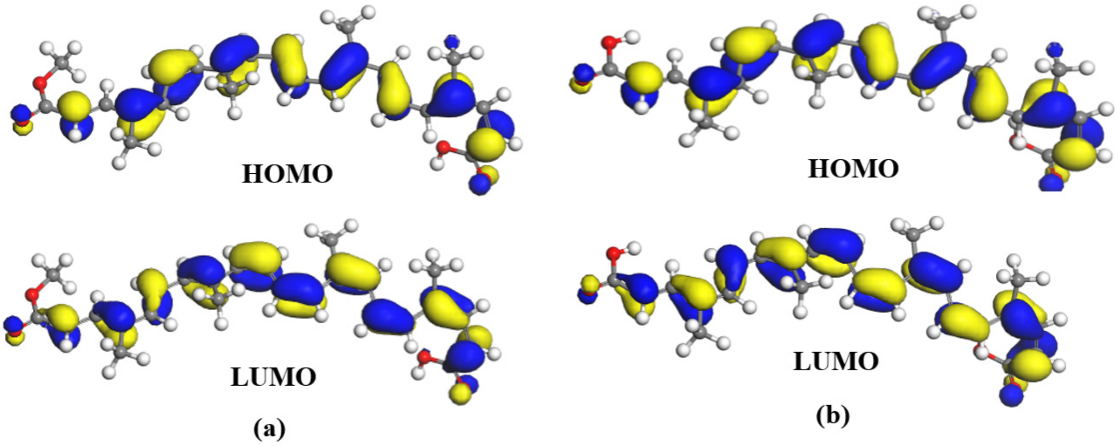

Figure 4. (**a**) HOMO and LUMO orbitals of bixin and (**b**) HOMO and LUMO orbitals of nobixin. (C = Grey; H = White; O = Red; Blue and yellow lobes represent negative and positive phases of the wave function, respectively].

Beyond the frontier orbital energies, additional quantum descriptors provide deeper insight into molecular reactivity and stability. Ionization energy (*IE*), which reflects the ease of electron loss, is slightly higher for norbixin, suggesting superior oxidative stability. Electron affinity (*EA*) trends indicate that norbixin also has a slightly stronger ability to stabilize excess electrons. Electronegativity (χ) values further show that norbixin is more electron-withdrawing than bixin, consistent with its increased polarity.

Table 2. HOMO, LUMO, and related quantum parameters for bixin and norbixin.

Parameter	**Bixin**	**Norbixin**
E_{HOMO} (eV)	–4.620	–4.848
E_{LUMO} (eV)	–3.152	–3.390
ΔE (eV)	1.468	1.458
IE (eV)	4.620	4.848
EA (eV)	3.152	3.390
χ (eV)	3.886	4.119
η (eV)	0.734	0.729
σ (eV^{-1})	1.362	1.372

The global hardness (η) and softness (σ) values reveal that bixin is relatively softer, which may favour faster electron transfer processes, while norbixin's slightly higher hardness could enhance chemical durability. Collectively, these quantum chemical findings affirm that both bixin and norbixin possess favourable electronic structures for efficient sensitization in DSSCs. While bixin may offer superior electron injection performance due to its greater softness and lower ionization energy, enhanced stability of norbixin could contribute to the long-term operational endurance of the device.

4. Conclusions

This study demonstrates the viability of *Bixa orellana* pigments, particularly bixin and norbixin, as promising sensitizers in dye-sensitized solar cells. The experimental results show that the acetone extract (a-AP) outperforms others in terms of power conversion efficiency, attributed to its broad absorption range and favourable electronic properties. Computational analysis further supports these findings, revealing that both bixin and norbixin possess the necessary electronic characteristics for effective electron transfer and light absorption. These results signify that *Bixa orellana* pigments offer a sustainable and efficient alternative for solar energy harvesting. Future studies should focus on optimizing extraction techniques, investigating co-sensitization strategies, and enhancing the stability and longevity of these natural sensitizers in practical DSSC applications.

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Author Contributions

Conceptualization, E.I.; Methodology, E.I. and M.U.; Software, E.I. and I.O.; Validation, E.I., I.O., R.U., S.U., M.U. and U.I.; Formal Analysis, E.I., I.O., R.U. and S.U.; Investigation, E.I., I.O. and R.U.; Resources, E.I., R.U., S.U., M.U. and U.I.; Data Curation,E.I., I.O. and R.U.; Writing—Original Draft Preparation, E.I., I.O., R.U., S.U., M.U. and U.I.; Writing—Review & Editing, E.I. and M.U.; Visualization, U.I.; Supervision, E.I.; Project Administration, E.I. and U.I.; Funding Acquisition, E.I. and U.I., please turn to the CRediT taxonomy for the term explanation.

Ethics Statement

Not applicable.

Informed Consent Statement

Not applicable.

Data Availability Statement

All data generated or analyzed during this study are included in this published article.

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Declaration of Competing Interest

The authors declare that there are no conflicting interest.

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