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Article

New Materials for Dye-Sensitized Solar Cells: Recent Advances, Efficiency Enhancements, and Future Prospects

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Abstract: Dye-sensitized solar cells (DSSCs) represent a promising third-generation photovoltaic cell. Due to their low cost, ease of fabrication, and flexible and transparent applications, DSSCs have been researched extensively. In this review, the development of materials used in DSSCs is examined. Recent innovations in photoanodes, sensitizers, electrolytes, and counter electrodes show that the properties of materials influence the power conversion efficiency (PCE), stability, and scalability of DSSCs. Various material combinations and their effects on the performance of DSSCs are compared, highlighting the research focus on solid-state and organic materials. Device architecture and nanotechnology contribute to the optimization of the DSSC's performance. It is necessary to enhance commercial viability so that DSSCs can be more widely used in building-integrated photovoltaics, wearable electronics, and energy-autonomous systems.

Keywords: DSSC, New materials, Solar cell, Photovoltaic, PCE, Dye

1. Introduction

The concern about growing global energy demand and climate change has led to extensive research on renewable energy technologies. Solar energy is one of the most promising resources due to its abundance and accessibility and has been widely used globally. At present, conventional silicon-based solar cells dominate the market. However, their high production cost, energy-intensive manufacturing, and rigidity have necessitated alternative technologies. Dye-sensitized solar cells (DSSCs), first introduced in 1991 [1], have emerged as a cost-effective and environmentally friendly alternative due to their photosensitizers to harvest light and semiconductors for charge transport.

DSSCs can be applied in applications requiring flexibility, semi-transparency, and indoor performance, as DSSCs perform well in low-light and high-angle light conditions, which are ideal for indoor environments or vertical architectural applications. However, challenges such as moderate efficiency, poor long-term stability, and issues with liquid electrolytes, including leakage and volatility, hinder the widespread use and commercialization of DSSCs. These limitations require continuous research to develop novel materials and device architectures to ensure the DSSC's performance and availability on the market.

Over the past several decades, significant progress has been made in enhancing the components of DSSCs, such as photoanodes, dyes, electrolytes, and counter electrodes, by incorporating advanced nanostructures, alternative chemicals, and hybrid systems. Based on existing knowledge, a review was conducted to examine the state-of-the-art DSSC materials and their integration, compare the performance of various combinations, and evaluate the role of emerging technologies, such as machine learning, in material discovery. This article provides a reference for the further development of DSSCs for widespread adoption in diverse applications.

2. History of DSSC Development

O'Regan and Grätzel demonstrated a 7% PCE using mesoporous TiO_2 and a ruthenium-based dye [1]. Their structure enabled a large surface area for dye adsorption and efficient light harvesting. Since then, DSSC architecture has evolved significantly, especially through the incorporation of nanomaterials, hybrid organic-inorganic dyes, and solid-state hole transport materials. In the early 2000s, spectral response was enhanced through the co-sensitization and engineering of new dyes, including ruthenium-based dyes, and natural dyes mixed with synthetic dyes such as Eosin Y, which have extended absorption in the visible and near-infrared regions [2]. At the same time, recombination losses were reduced, which led to surface passivation strategies and enabled compact layers between TiO_2 and fluorine-doped tin oxide (FTO) glass. Quasi-solid and solid-state electrolytes were developed to prevent electrolyte leakage and minimize volatility. The electrolytes ensured the device's stability under thermal cycling and illumination [3]. In addition, carbon-based materials and conductive polymers for counter electrodes enabled low-cost alternatives to platinum for DSSCs. Recently, perovskite materials, tandem configurations, and machine-learning-aided design have been integrated into DSSCs. AI algorithms enable the fast discovery of new dyes, optimization of photoanode structures, and prediction of interactions among DSSC components [3]. These advancements lead DSSCs to be used in niche applications where flexibility, transparency, and aesthetic integration are crucial, such as building-integrated photovoltaics (windows, facades, and skylights), wearable electronics (smart clothing and portable devices), indoor energy harvesting (wireless sensors and IoT devices), automotive industry (sunroofs and tinted windows), aerospace and military (lightweight, portable power solutions for remote operations).

3. Materials for DSSCs

Each component of the DSSC contributes significantly to the overall efficiency and stability of the device. Innovations in material selection and structural optimization have improved the performance of DSSCs and led to their broader applications (Table 1).

3.1. Photoanode Materials

The photoanode is a key to electron collection and transport efficiency. Conventionally, nanocrystalline TiO_2 deposited on FTO glass is used due to its favorable conduction band alignment, high surface area, and chemical stability. To enhance charge transport, 1D and 3D TiO_2 nanostructures, nanostructures, such as nanotubes, nanowires, and hierarchical assemblies, have been developed. These morphologies facilitate directed electron transport and reduce recombination. Doping TiO_2 with elements, including niobium (Nb), tantalum (Ta), or fluorine (F), increases the conductivity and the Fermi level of DSSCs [5]. Incorporating graphene and reduced graphene oxide (rGO) into TiO_2 matrices also improves electron mobility and mechanical flexibility.

ZnO and SnO_2 are promising alternatives to TiO_2. ZnO has a similar band structure to TiO_2 and allows for faster electron mobility, but it suffers from chemical instability and dye degradation under prolonged exposure [6]. SnO_2 offers higher electron mobility (up to 100–300 cm^2/Vs) compared with TiO_2 (up to 1 cm^2/Vs). However, it has higher recombination rates unless passivated [7]. Recently, researchers have applied composite photoanodes that blend TiO_2 and SnO_2 and incorporate buffer layers such as Nb_2O_5 to manage band alignment and minimize back electron transfer.

3.2. Sensitizer Dyes

Dyes act as the primary light absorbers and electron injectors in DSSCs. The dye affects the spectral response, charge injection efficiency and device stability. Ruthenium complexes, including N3, N719, and Z907, are widely used in DSSCs due to their long-term stability and strong absorption in the visible spectrum [8]. However, their high cost and the presence of rare metals limit the scalability of DSSC manufacturing using ruthenium complexes. Metal-free organic dyes have been given significant attention for their tunability, high molar extinction coefficients, and ease of synthesis. Donor–*π*–acceptor (D–*π*–A) structures, such as those based on indoline, triphenylamine, or carbazole, offer broad absorption and customizable energy levels [9]. As natural pigments, porphyrins and phthalocyanines are used as dyes to absorb light in the near-infrared region. Their PCEs exceed 12% when co-sensitized with complementary dyes [10]. Co-sensitizing photoanodes with two or more dyes expands light absorption ability and improves electron injection efficiency. For example, a broad-spectrum dye with a high open-circuit voltage (Voc) is used to balance photocurrent and voltage [10]. Although not yet competitive in efficiency, dyes extracted from fruits and flowers are used, as they enable low toxicity and biodegradability. Natural dyes are mainly used for educational or indoor applications at present.

3.3. Electrolytes

The electrolyte is responsible for dye regeneration and ion transport. Traditional DSSCs use an iodide/triiodide redox couple in an organic solvent like acetonitrile. While effective, these electrolytes are volatile and corrosive.

Ionic liquids are salts in liquid form at room temperature, offering non-volatility, thermal stability, and good ionic conductivity. They suppress evaporation and extend the device's lifetime under thermal stress [11]. Gel polymer electrolytes (GPEs) based on polyvinylidene fluoride-co-hexafluoropropylene (PVDF-HFP), polymethyl methacrylate (PMMA), or polyethylene oxide (PEO) matrices combine solid-state integrity with liquid-like ion mobility. They improve mechanical stability and reduce leak resistance, which is critical for flexible or wearable DSSCs [13]. Solid-state hole transport materials (HTMs), such as 2,2′,7,7′-tetrakis(N,N-di-p-methoxyphenylamine)-9,9′-spirobifluorene (Spiro-OMeTAD) and Cu-based complexes, replace the liquid electrolyte altogether, enabling solid DSSCs with improved sealing and longevity [12]. However, crystallization, poor pore filling, and low conductivity are issues to be solved. To overcome the limitations of I^-/I_3^-, alternative redox mediators such as cobalt complexes, copper complexes, and ferrocene derivatives have been researched to increase their Voc and recombination rates [13].

3.4. Counter Electrode Materials

The counter electrode is used to catalyze the reduction of the redox mediator and completes the electrical circuit. Pt is widely used due to its highly catalytic and stable capability. It is regarded as the standard, but Pt is expensive and sensitive to iodine corrosion [8]. Carbon-based materials, including graphene, carbon nanotubes (CNTs), and activated carbon, offer excellent conductivity and corrosion resistance. Their low cost and tunable morphology make them ideal for flexible and large-area applications [14]. Conducting polymers, such as poly(3,4-ethylenedioxythiophene (PEDOT) and polyaniline (PANI), offer flexibility, easy processing, and decent catalytic performance. Their mechanical properties are advantageous for roll-to-roll printing and flexible DSSCs [15]. Transition metal compounds, such as sulfides and selenides of cobalt, nickel, and molybdenum (e.g., NiS, MoS_2), are gaining traction as cost-effective, earth-abundant counter electrodes with high electrocatalytic activity [16].

Table 1. DSSC materials, roles, and advancements.

Component	Role in DSSC	Conventional Materials/Approaches	Innovations/Alternative Materials
Photoanode	Electron collection and transport	Nanocrystalline TiO_2 on FTO glass	1D & 3D TiO_2 nanostructures (nanotubes, nanowires, hierarchical assemblies); Doping TiO_2 (Nb, Ta, F); Graphene/rGO in TiO_2; ZnO; SnO_2; TiO_2/SnO_2 composites with buffer layers (e.g., Nb_2O_5)
Sensitizer dyes	Primary light absorbers and electron injectors	Ruthenium complexes (N3, N719, Z907)	Metal-free organic dyes (D-π-A structures: indoline, triphenylamine, carbazole); Porphyrins; Phthalocyanines; Co-sensitization; Natural dyes (fruits, flowers)
Electrolytes	Dye regeneration and ion transport	Iodide/triiodide redox couple in organic solvent (acetonitrile)	Ionic liquids; Gel polymer electrolytes (GPEs: PVDF-HFP, PMMA, PEO); Solid-state Hole Transport Materials (HTMs: Spiro-OMeTAD, Cu-based complexes); Alternative redox mediators (cobalt, copper complexes, ferrocene derivatives)
Counter electrode	Catalyzes redox mediator reduction, completes circuit	Platinum (Pt)	Carbon-based materials (graphene, CNTs, activated carbon); Conducting polymers (PEDOT, PANI); Transition metal compounds (sulfides/selenides of Co, Ni, Mo, e.g., NiS, MoS_2)

4. Efficiency of DSSCs

Efficiency in DSSCs is influenced by the interplay between all components: the photoanode, dye, electrolyte, and counter electrode. A performance metric to evaluate the efficiency is PCE, which depends on the short-circuit current density (Jsc), Voc, and fill factor (FF).

Ruthenium-based DSSCs show PCEs of up to 11–12% under standard Air Mass 1.5 solar spectrum (AM1.5) when paired with optimized TiO_2 and Pt electrodes using I^-/I_3^- electrolytes [8]. Devices using N719 with liquid electrolyte are used as a benchmark for comparison. Organic dyes or metal-free dyes based on D–π–A architecture, such as Y123 and D35, have achieved PCEs of 10–13% when co-sensitized and matched with cobalt redox shuttles and NiS counter electrodes [9,10]. YD2-o-C8 and other porphyrin dyes have reached PCEs of up to 13% with cobalt electrolytes, showcasing their potential for near-infrared harvesting [10]. Solid-state DSSCs have lower PCEs (7–10%) due to incomplete pore filling and poor hole mobility in solid hole transport materials (HTMs), such as Spiro-OMeTAD, although they do not have electrolyte leakage issues [12].

In DSSCs, graphene or CNT electrodes are widely used as they offer better long-term stability and are well-suited for flexible applications, although the PCEs remain 7–9% [14]. DSSCs with copper-complex redox shuttles and ionic liquid-based electrolytes show PCEs of 9–11% while demonstrating enhanced stability under prolonged illumination and elevated temperature [13]. Laboratory-scale DSSCs have achieved up to 14.3% PCE when using co-sensitized dyes, optimized cobalt complexes, and hierarchical TiO_2 structures [2]. However, reproducibility and long-term performance must be enhanced for commercialization.

Table 2. DSSC performance summary.

DSSC type	Key component	PCE
Ruthenium-based DSSC	N719 dye, optimized TiO_2 and Pt electrodes, I^-/I_3^- electrolytes	Up to 11–12%

Organic/metal-free dyes	Y123 and D35 (D–π–A architecture), co-sensitized, cobalt redox shuttles, NiS counter electrodes	10–13%
Porphyrin dyes	YD2-o-C8, cobalt electrolytes	Up to 13%
Solid-state DSSCs	Solid hole transport materials (HTMs) like Spiro-OMeTAD	7–10%
Graphene/CNT electrodes	Graphene or CNT electrodes	7–9%
Copper-complex redox shuttles	Copper-complex redox shuttles, ionic liquid-based electrolytes	9–11%
Laboratory-scale (co-sensitized) DSSC	Co-sensitized dyes, optimized cobalt complexes, hierarchical TiO_2 structures	Up to 14.3%

5. Future Development

Future research in DSSCs aims to address efficiency, stability, and scalability to unlock wider commercial and environmental applications.

Tandem DSSCs stacked or side-by-side with perovskites or organic photovoltaics are effective in the absorption spectrum and increase PCE to higher than 15% [17]. These systems require transparent counter electrodes and careful energy level alignment to function efficiently. Integration into wearables and building-integrated photovoltaics demands lightweight, flexible substrates, such as PET and ITO-coated plastics. Recent advances in roll-to-roll printing and metal mesh electrodes enable scalable fabrication of DSSCs for such applications [15].

Machine learning models have been applied to predict dye absorption properties, charge transfer rates, and electrolyte compatibility based on molecular descriptors [4]. AI-assisted materials informatics is streamlining the design of new dyes, redox couples, and nanostructures by reducing reliance on trial-and-error experimentation. However, it is required to find and develop stable dyes resistant to photodegradation, thermally stable electrolytes (e.g., quasi-solid or ionic liquid), and robust encapsulation methods. For wide use and commercialization, DSSCs need to have higher initial PCEs than 90% and retention over 1,000 hours of continuous operation under light and temperature cycling. With increasing interest in green electronics, biodegradable dyes, and water-based electrolytes are being researched. While their efficiencies are lower (1–3%), their benign nature makes them ideal for disposable or low-cost applications in agriculture, remote sensing, or educational tools [18]. Companies, including G24 Power and Exeger, are developing commercial DSSCs for indoor energy harvesting. However, it is crucial to enhance reproducibility, lower the cost per watt, and improve durability, which necessitates ongoing collaboration between academia and industry.

To enhance reproducibility, machine learning (ML) algorithms are used to model and predict optimal fabrication parameters [19]. Using ML is expected to address the batch-to-batch variability of materials such as dyes, electrolytes, and mesoporous TIO_2 photoanodes. Standardized screen-printing techniques for TiO_2 layers and dye-loading procedures have demonstrated enhanced consistency across large-scale production [20]. Furthermore, pre-synthesized ruthenium-based dyes and metal-free organic dyes with high purity have shown reduced variation in photoresponse among fabricated cells [21].

To lower the cost per Watt, carbon-based electrodes and transition metal sulfides are used, as they enable material substitution and process innovation. Platinum-based counter electrodes, while efficient, are expensive, but significantly reduce electrode cost while maintaining catalytic activity [22]. Natural dyes extracted from anthocyanins and betalains were identified to be promising for eco-friendly, low-cost sensitizers despite their tradeoffs in longevity and efficiency [3]. Additionally, roll-to-roll manufacturing and printing techniques have been explored to reduce production costs by scaling up manufacturing processes [23].

DSSCs suffer from electrolyte volatility and photochemical degradation. Recent advancements in quasi-solid and solid-state electrolytes, when incorporating ionic liquids and gel polymer matrices, have significantly improved device stability while retaining ionic mobility. Encapsulation technologies using ultraviolet (UV)-stable polymers and advanced sealing methods have extended device lifetime under real-world conditions. Moreover, the development of hydrophobic dyes and surface treatments enhances resistance to moisture-induced degradation. Several DSSCs have demonstrated operational stability beyond 10,000 hours in accelerated aging tests [24].

6. Conclusion

DSSCs have evolved considerably since their inception, with innovations in each component leading to incremental gains in performance and functionality. TiO_2 remains the dominant photoanode, while organic and porphyrin dyes challenge ruthenium complexes in efficiency. Electrolyte developments and counter-electrode alternatives offer pathways to safer, more flexible devices. As ML accelerates material discovery and improves reproducibility, DSSCs are expected to contribute to decentralized and integrated solar energy systems. The recent convergence of material science, predictive modeling, and scalable manufacturing methods is progressively overcoming the longstanding limitations of DSSCs. While efficiency remains modest compared with traditional silicon photovoltaics, innovations focusing on reproducibility, cost reduction, and durability are positioning DSSCs as viable options for niche applications, including building-integrated photovoltaics and indoor energy harvesting. Future efforts are still necessary to enhance the long-term stability, sustainability, and industrial scalability of DSSCs.

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