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Titanium Dioxide Band-Gap and Interfacial Energy-Level Engineering in Dye-Sensitized Solar Cells – A Narrative Review

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ABSTRACT

The wide band gap of TiO_2, its chemical stability, high specific surface area of mesoporous films and favourable electron-accepting states enable efficient dye-sensitization, made TiO_2 preferred photoanode semiconductor in dye-sensitized solar cells (DSSCs). But, recent studies demonstrate that optical band gap alone is not sufficient to explain the role of TiO_2 in photovoltaic (PV) application. All the above methods can influence the position of the conduction band, electron density, trap distribution, dye adsorption, electron transport and recombination at the same time. This review, thus, considers band-gap engineering as one of many aspects of interfacial energy-level engineering. The current literatures are coupled with existing mechanism studies to examine the impact of recent changes on injection, transport, recombination and device output. The special cases of matched control, dye loading, electrolyte effects and difference between optical-gap shifts and actual changes in operating energy alignment are discussed in particular detail. In recent years, the use of In-, Ag-, Mg-, Al- and rare-earth-doped TiO_2 has been reported, as well as TiO_2 that is also doped with Ti^{3+}, one-dimensional and hierarchical architectures, and TiO_2/rGO, TiO_2/MoS_2-rGO and TiO_2/g-C_3N_4 composites. Single-layer/bilayer TiO_2 has also been reported. This review suggests that the best design strategy is not to maximize band-gap narrowing or conductivity, but to design an optimized interface between TiO_2, dye and electrolyte that ensures dye loading, an adequate driving force for electron injection, transport and low back-electron transfer, and stability during operation.

Keywords: TiO_2; DSSCs; band-gap engineering; energy-level alignment; interface engineering.

1.0 INTRODUCTION

The main characteristics of dye-sensitized solar cells are that light is absorbed by a dye and the dye is excited, the excited dye injects an electron into semiconductor, the former gets oxidized in the process, and the oxidized dye is regenerated by a redox mediator, as electrons pass through the oxide network to transparent conducting substrate. In the past, anatase form of TiO_2 has been applied as a reference photoanode, since it is chemically stable and has high area mesoporous structure, with more or less appropriate accepting states. Key factors in dye-to-TiO_2 injection and transport and recombination processes were identified in classic DSSC studies and further research demonstrated that the microscopic structure of the oxide network (O'Regan & Grätzel, 1991; Hagfeldt et al., 2010; Muñoz-García et al., 2021), the nature of states in the oxides, and the surface chemistry of TiO_2 play a major role.

In the past few decades, especially since 2024, many other linked processes apart from bandgap modifications have been reported to influence performance of DSSC upon modification of TiO_2. The electronic structure of TiO_2 can be modified by change of dopant composition, defect structure, crystallographic features, morphology and surface chemistry which can have significant influence on dye-TiO_2 interface, charge injection, electron transport and recombination (Addae et al., 2026; Rahman et al., 2023). The apparent optical band gap is not a necessary condition for an improved electron injection interface as the shift might be attributed to defects and disorder in the structure or to change of composition. Similarly, improved efficiencies reported for PV cells cannot always be directly linked to a change in PV material band-gap, but rather than to enhanced dye adsorption, light scattering, electron transport and the suppression of interfacial recombination and changes in electrolyte interactions can all have a significant effect on device efficiencies (Ashrafuzzaman et al., 2025; Premkumar et al., 2024). It is critical to distinguish these effects and give insight into how modification of TiO_2 affects the alignment of its energy levels with those of N719 or energy-level alignment of two nanocrystals that are close to each other in energy (Khairudin et al., 2026; Sharipbaev et al., 2026;Khan et al., 2021). It is essential to differentiate these effects and understand the changes in energy-level alignment or changes in the alignment of the two nanocrystals that are close in energy after the modification of TiO_2, which ultimately determine the operation of the DSSC.

2.0 LITERATURE APPROACH

This is a narrative review rather than a formal systematic review. The updated search emphasized peer-reviewed studies and reviews published from 2021 to 2026, with particular attention to TiO_2 photoanodes, DSSC energy-level alignment, doping and defect engineering, morphology/facets, compact and passivation layers, heterostructures, dye adsorption, charge-transfer measurements and stability (Markose et al., 2023; Khan et al., 2021). Publisher records and DOI metadata were used to verify bibliographic details of the added literatures. Foundational papers were retained where they are necessary for interpreting mechanisms. Efficiencies are not pooled because reported dyes, electrolytes, active areas, illumination

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conditions, film thicknesses and device architectures differ substantially.

3.0 TiO_2 ENERGETICS: WHY THE OPTICAL BAND GAP IS NOT ENOUGH

Anatase TiO_2 is referred to as a wide-band-gap semiconductor, the optical gap of which is close to 3.2 eV. In the case of a DSSC, however, the energy levels that play a role are the energy of the conduction band edge, energy levels localized below the conduction band, the energy at the excited state oxidation potential of the dye, and the quasi-Fermi energy of the electrons under illumination and the energy level of the electrolyte. Enabling atmosphere for electron injection is provided by the energetic driving force and electronic coupling. Surface protonation, adsorbed ions, molecular dipoles, exposed crystal facets, defects, and dopants can alter the interfacial potential, even when they produce only small changes in the optical band gap (E_{opt}) (Roose et al., 2015; Muñoz-García et al., 2021).

Experimental evidence is in for this separation is recent. All the doped samples showed improvement in their carrier concentration, charge-transfer resistance, and the highest doped sample showed efficiency of 8.62% as compared to 5.57% for the undoped sample. The improvement was attributed to the improvement of electronic conductivity and suppression of recombination rather than just a red shift by the authors (Ayaz et al., 2024). A change in the optical and electronic behavior and a change in the transport impedance of the electron lifetime and VOC were also observed in the case of Ag-doped TiO_2 and Mg-doped compact TiO_2 respectively (Sharipbaev et al., 2026, Pervaiz *et al*., 2024; Deng et al., 2021). The examples illustrate the need to consider 'band-gap engineering' in a broader context of electronic and interfacial changes that are coupled.

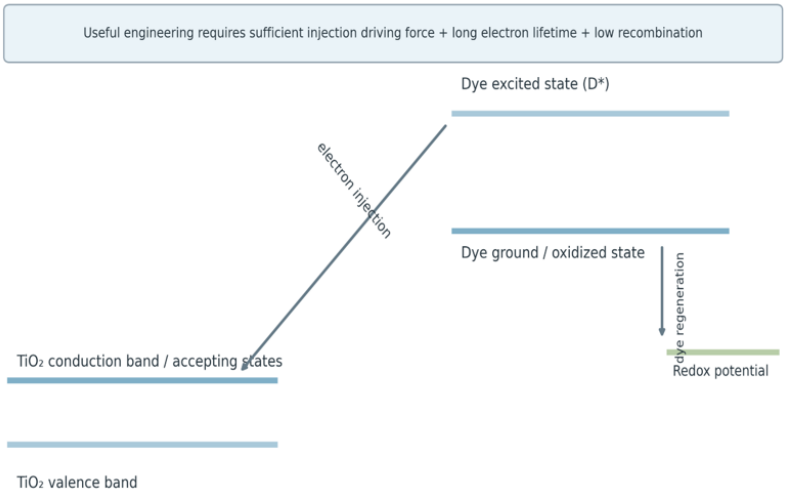

Figure 1. Conceptual energy landscape for a TiO_2-based DSSC. A useful modification must balance dye-to-TiO_2 injection, electron transport and recombination suppression rather than maximize a single band shift.

4.0 DOPING AND DEFECT ENGINEERING

Doping causes changes in the density of carriers, crystallinity, population of defects, conductivity and surface potential. These effects can be both positive and negative and are dependent upon the dopant, its concentration, where and how it was synthesized. Previous studies have shown that band structure and trap states can be modified by doping with TiO_2, and it is problematic to compare since different defect chemistries can be produced by various synthetic methods (Markose et al., 2023; Roose et al. 2015). A recent study by DSSC offers a number of helpful examples, in Table 1, has summary of recent TiO_2 doping and surface-modification techniques that have enhanced the performance of DSSCs by boosting the carrier density, reducing the interfacial resistance, prolonging the lifetime of electrons, loading more dye molecules, and suppressing electron recombination are listed. It does note, however, that these benefits are highly dependent on type of dopants, concentration, distribution, compact-layer properties and associated structural changes. Optical-gap shifts reported or efficiency gains are therefore not enough for establishing mechanism; matched structural, electrochemical and photovoltaic controls are needed.

Table 1: Representative recent TiO_2 doping/defect strategies and the mechanistic interpretation required

Modification	Recent evidence	Ref.	Likely mechanism	Important caution
In-doped TiO_2	8.62% PCE; lower charge-transfer resistance.	Ayaz et al. (2024)	Higher carrier density/conductivity; lower interfacial resistance.	Excess dopant can introduce scattering/recombination centres.
Ag-doped TiO_2	Optical/electronic modification; reported 6.31% PCE.	Ramadhani et al. (2024)	Defect/electronic-state modification and reduced recombination.	Optical-gap change alone does not establish the mechanism.

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Mg-doped compact TiO_2	Higher V_OC and electron lifetime reported; optimized device reached 7.843% PCE.	Zhang et al. (2025)	Compact-layer passivation; altered transport and recombination.	Compact-layer thickness and conductivity must be controlled.
Ti^{3+}-rich/faceted TiO_2	8.82% PCE; 22.7% improvement versus the reference.	Li et al. (2024)	Modified band structure, higher dye loading and lower recombination.	Ti^{3+} concentration and surface location are critical.
Al-doped TiO_2	Optimized loading was associated with porosity, crystallinity and dye loading; optimized device reported 1.34% PCE.	Abiram et al. (2025)	Combined structural and electronic effects.	Dopant concentration changes several variables simultaneously.
Rare-earth-doped TiO_2	2026 study of Ho^{3+}, La^{3+}, Er^{3+} and Yb^{3+}; dopants modified optical, structural and surface properties.	Caliskan et al. (2026)	Modified photoelectrochemical properties; dopant-specific structural, surface and charge effects.	Dopant-specific effects require matched controls.

Li et al (2024)introduced Ti^{3+} within TiO_2 to improve photoanode electron transport performance in DSSCs, this introduction on exposed (001) anatase surfaces and a modification photoanode showed increased dye loading, lower recombination and an 8.82% PCE. This result supports an idea that defect engineering can be beneficial when the defect state is controlled and coupled to a favorable surface structure. It does not justify that treating Ti^{3+} or oxygen vacancies as universally beneficial as excessive localized states can act as trapping/recombination centers.

5.0 PHASE, MORPHOLOGY AND CRYSTALLOGRAPHIC-FACET ENGINEERING

The phase composition of TiO_2 affects the ability of dye molecules to be adsorbed to the surface, the conductivity of electrons between the particles and in the bulk, the chances for recombination and the cell performance (Johnson et al., 2026). The nanostructure, porosity, particle connectivity and exposed crystal facets affect dye adsorption, the conductivity of electrons between the particles and in the bulk, recombination and cell performance (Joshy et al., 2022; Kaur et al., 2023). Mesoporous TiO_2 should also have a large amount of dye loading capability, connected electron pathways, high optical thickness and penetration depth for an electrolyte. So, in practice, the morphology is coupled with the energetics in the DSSC technology. While the nanoparticle films have better surface area, they also have numerous boundaries of nanoparticles, nanorods, nanotubes and nanowires can offer more direct paths for transportation, but they might sacrifice a certain amount of surface area. These conflicting requirements have been found to be well balanced with hierarchical and one-dimensional architectures in recent reviews and studies (Srivastava et al., 2025; Korir et al., 2025; Lana et al., 2024; Huang et al., 2021).

Experimental studies in the last few years also show that different output and structure can be achieved by varying the phase composition and the calcination history of the devices. When tri-phase TiO_2 was studied, it was found that the anatase/rutile/brookite (A/R/B) ratio increased with the increase in calcination temperature and the best PCE was obtained at calcination temperature of 600 °C (Kanwal et al., 2024). To overcome this, in 2024 a study on the fiber-shaped DSSC was published and this inspired the development of the flower-like architecture of TiO_2 for DSSC (Abdulsalami et al., 2026;Srivastava et al., 2025; Lin et al., 2024). Recently, Srinivasan et al.(2026) reported the anatase facet selective TiO_2 material with 6.6% efficiency of PCE due to high number of adsorption sites for the dye and high charge separation/transit. These results do not only constitute additional evidence of facet engineering but also indicate the necessity of a simultaneous measurement of the dye loading, film thickness, scattering and crystallinity.

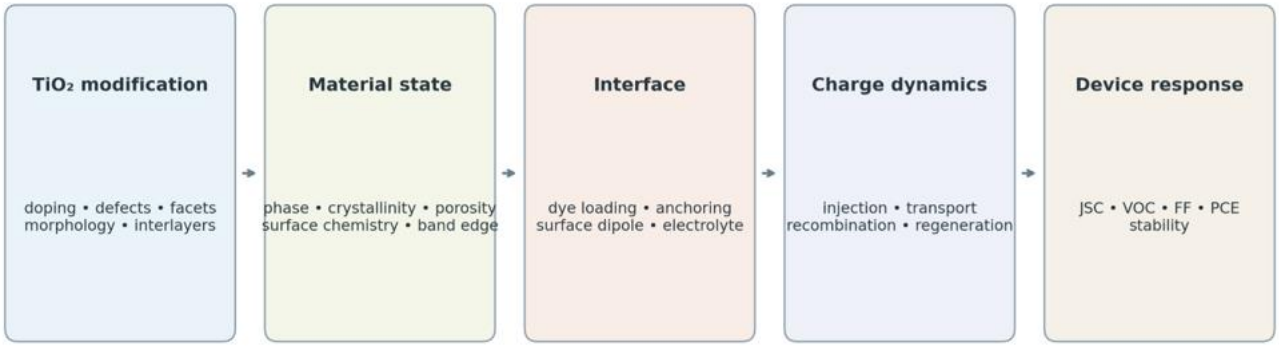

Figure 2. Causal chain linking TiO_2 engineering to DSSC performance. The figure emphasizes why a photovoltaic change should not be assigned to a band-gap shift without intermediate evidence.

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6.0 ONE-DIMENSIONAL AND HIERARCHICAL TiO_2 ARCHITECTURES

The one-dimensional architecture of TiO_2 (1D TiO_2) is beneficial to minimize number of interparticle junctions and facilitates the direction electron transport. The drawback of their use is that they tend to have lower internal surface area than do nanoparticle films. Recent review articles found that most promising designs are not necessarily just 1D – hierarchical designs can be a combination of a high area scaffold of nanoparticles and less direct transport pathways (Lana et al., 2024; Lin et al., 2024; Pervaiz et al., 2024). The most important variables are dye uptake, connectivity, electron diffusion, scattering and recombination.

Therefore, comparisons should be made between thickness matched layers and should include measurements of dye adsorption, IPCE, optical transmission/reflectance, impedance and/or transient transport, and statistics of the device. The multi-variable behaviour is seen in TiO_2/MoS_2-rGO composite where MoS_2 is associated with the charge transport and rGO is associated with the porosity, which resulted in an improved PCE (Hemavathy et al., 2026; Amini et al., 2025). This is an informed improvement for DSSC technology, but it is important to separate contribution of each of its components experimentally before assigning gain to each band-alignment mechanism.

7.0 HETEROSTRUCTURES, COMPOSITES AND INTERFACIAL PASSIVATION

Introduction of new electronic paths or passivation of unprotected surfaces, changing optical response, or creating an interface band offset are all possible uses of TiO_2 composites. TiO_2/rGO, TiO_2/g-C_3N_4 and TiO_2/MoS_2/rGO systems have been recently researched (Ali et al., 2025; Sardar et al., 2024). The performance reported by studying TiO_2/g-C_3N_4, has been attributed to type-II band alignment and low recombination rate of TiO_2/g-C_3N_4 (Hemavathy *et al*., 2026;Amini et al., 2025). If the amount of g-C_3N_4 is too high, it would adversely affect the TiO_2 network, and this would reduce the transport (Amini et al., 2025). A typical type of composite photoanodes is a non-monotonic behavior. On the other hand, there are compact TiO_2 layers and ultrathin passivation layers at the TCO/photoanode/liquid interface. These can block direct contact by the electrolyte, decrease recombination, but if these are too resistive or thick, they will decrease the ability of the electrons to be collected or the dye to be adsorbed. Based on the literatures, it is observed that issue of passivation is more than just a barrier layer issue, it is also a tunneling and surface chemistry issue (Ju*et al*., 2026; Roy *et al*., 2023).

Table 2 compares TiO_2 engineering strategies for improving charge transport, energy-level alignment, light harvesting, and recombination control in DSSCs. It shows that doping, defect control, tailored morphology, facet engineering, conductive composites, heterostructures, and passivation layers can enhance electron collection and photovoltaic performance, but each introduces trade-offs such as deep traps, reduced dye loading, added interfacial resistance, aggregation, or blocked transport pathways.

Table 2. Mechanistic comparison of major TiO_2 engineering strategies.

Strategy	Primary target	Potential gain	Main trade-off / control
Doping	Carrier density, band edge, defects	Transport or recombination control	Dopant concentration; matched film morphology
Ti^{3+}/defect control	Trap distribution, conductivity	Faster transport; altered surface energetics	Deep traps and instability
1D/hierarchical TiO_2	Connectivity + optical path	Reduced transport losses	Lower dye-loading area
Facet engineering	Surface chemistry and adsorption	Dye loading; charge separation	Facet-dependent synthesis reproducibility
rGO/MoS_2 or carbon composites	Electron pathways/porosity	Lower transport resistance	Additional interfaces; aggregation
g-C_3N_4 heterostructure	Band offsets/recombination	Charge separation; broader absorption	Excess phase can block TiO_2 network
Compact/passivation layer	Substrate and surface recombination	Higher electron lifetime/VOC	Series resistance; tunneling distance

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8.0 DYE ADSORPTION, ANCHORING AND ELECTROLYTE EFFECTS

They form an electronic bridge (not a passive coating) between dye and TiO_2. Electronic coupling and sensitized sites are influenced by the geometry of the anchor, the hydroxylation of the surface, the acidity and the aggregation of the facets. Though measurements were conducted under dry conditions of the dye coated electrodes, in situ neutron reflectivity was performed to show that constituents of the electrolyte can invade the dye self-organization and alter the interfacial structure, providing an explanation for this. The ab initio molecular-dynamics simulation also revealed that dye structure has an impact on the dynamics of charge transfer at the interface (He et al., 2021).

Recently, adsorption control was shown to be an effective way to alter the balance of transparency and photocurrent for recent DSSC work with transparent DSSCs. Therefore, if an increase in J_{SC} is obtained by a TiO_2 treatment, the analysis should be able to identify whether the amount of dye adsorbed, the orientation of the adsorbed dye, the increased optical scattering or the improved injection yield is responsible for the increase in J_{SC}. The quantitative measurement of dye loading should, thus, be used preferably in conjunction with the absorbed-photon-normalized photocurrent or IPCE.

9.0 TRANSPORT, RECOMBINATION AND PHOTOVOLTAIC METRICS

The connectivity of particles, occupation of the traps and thickness of the film and electron number are the factors that govern the electron transport through mesoporous TiO_2. The parameters obtained by fitting the EIS results can be used to estimate recombination resistance and chemical capacitance, but each of these parameters depends on the condition and thus is not necessarily determined by the other parameters. The complementary information on transport and recombination can be obtained from intensity-modulated photocurrent or photovoltage and transient optical methods. Photovoltage can increase due to suppression of recombination, change in the TiO_2 conduction band edge, change in electrolyte redox potential, or change of quasi-Fermi level of an electron. A reduced optical gap may influence light absorption and interfacial energetics, but its effect on J_{sc} *or* V_{oc} depends on the accompanying changes in charge injection, transport, and recombination. Several factors can affect the fill factor, such as series resistance, counter-electrode reaction rate and shunt pathways and mass transport. Therefore, the assessment of a TiO_2 mechanism needs to be made from the entire J–V curve along with supporting evidence.

To interpret the common DSSC performance changes, without over assigning mechanisms, an interpretation framework is presented in Table 3. It highlights several possibilities of the optical gap, current density, voltage, fill factor, efficiency and electron lifetime changes coming from several structural, optical, interfacial and electrolyte factors. The individual observations should then be matched with complementary measurements, however, before it can be said that the result is due to a certain type of engineering mechanism for the TiO_2.

Table 3. Interpretation matrix for common DSSC observations.

Observation	Possible causes	Measurements needed before assigning mechanism
Lower apparent optical gap	Doping, defects, phase change, disorder, scattering	UV–Vis/DRS + XRD/XPS/EPR + sensitized-electrode/IPCE
Higher JSC	More dye, stronger absorption/scattering, better injection, transport	Dye loading + IPCE + optical spectra + transient/EIS
Higher VOC	Lower recombination, band-edge shift, electrolyte shift	Dark current + EIS/lifetime + band/work-function data
Higher FF	Lower series resistance, better collection, CE/electrolyte changes	Series resistance + CE controls + EIS + matched device assembly
Higher PCE	Any combination of JSC, VOC and FF	Replicated J–V + IPCE + mechanistic measurements
Longer electron lifetime	Lower recombination or altered capacitance/fit regime	EIS/IMVS + matched electron density/illumination

10.0 CHARACTERIZATION FRAMEWORK AND REPORTING STANDARDS

For a comprehensive TiO_2-engineering study, the order of the steps shown in Figure 3 is recommended. The materials should be initially confirmed as a material change by performing phase, morphology and chemical state characterization. Second, complementary energy-level and adsorption measurements of the dye loaded, electrolyte contacted interface should be done. Third, it is important to measure the charge dynamics under matched illumination and at similar electron density (if possible). Finally, replicated PV and stability data should be used to confirm whether or not there will be a repeatable PV and stability benefit afforded by the proposed mechanism.

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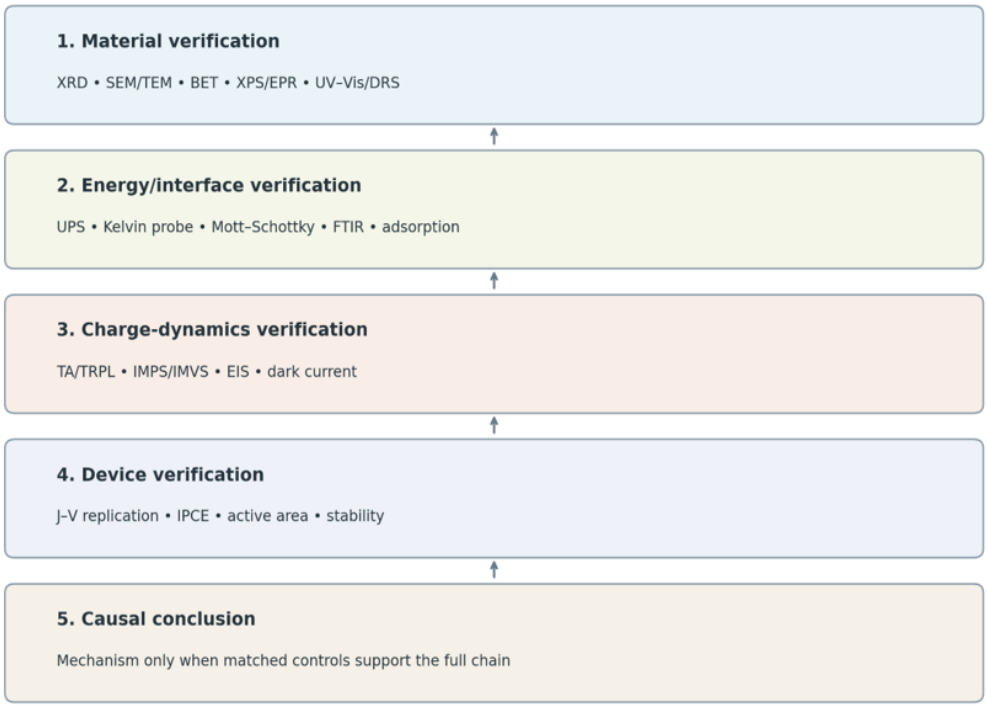

Figure 3. Evidence-based verification framework for establishing causal mechanisms in TiO_2-engineered DSSCs.

In the table 4 below, the minimum evidence and controls that are necessary for making claims about TiO_2 engineering in DSSCs are defined. These include assertions of band-edge shifts, defect or facet engineering, passivation, composites, and stability which must all be accompanied by complementary material, interfacial, kinetic, and device measurements with a set of well-matched reference systems.

Table 4. Minimum evidence needed to support common mechanistic claims.

Claim	Minimum evidence set	Preferred control
Band-edge shift improves injection	UPS/Kelvin probe or Mott–Schottky + transient injection + dye energetics	Undoped TiO_2 with matched dye loading and thickness
Defect engineering improves transport	XPS/EPR + transport/lifetime + recombination analysis	Defect concentration series
Facet engineering improves performance	HRTEM/XRD facet evidence + dye loading + transport/IPCE	Commercial P25 or identical synthesis without facet-control agent
Passivation suppresses recombination	Dark current + EIS/lifetime + adsorption/injection evidence	Chemically similar inactive interlayer
Composite improves charge separation	Band/interface characterization + transient/EIS	Individual components and physical mixture
Stability is improved	Repeated J–V/IPCE under defined light/temperature/electrolyte conditions	Unmodified reference aged in parallel

11.0 INTEGRATED DESIGN RULES AND RESEARCH PRIORITIES

It is not only the energy landscape of the dry dye/TiO2 interface that should be considered in charge-transfer processes in DSSCs but also the operating dye/TiO_2/electrolyte interface. Thus, the Tauc derived optical band gap cannot be directly used as an indication of conduction band location and/or the injecting force for an electron. Special emphasis needs to be placed also on the concentration and the chemical state of the defects: if defects increase the conductivity of the material at relatively low concentrations, an excess of defects could result in a significant increase of charge recombination. Likewise, it is necessary to consider the morphology of TiO_2 films within a set of interconnected properties that control the amount of dye absorbed, the distance over which the electrons have to travel to reach the dye, light scattering, pore accessibility and particle-to-particle connectivity instead of considering an individual property.

The use of the compact or passivation layers also needs optimization as the beneficial effect is critically dependent on the layer resistance being sufficiently low and the right 'tunneling distance' to collect the electrons productively. Comparisons should thus be made under similar conditions

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such as film thickness, dye loading, sintering history, electrolyte composition, illumination conditions and active area between the modified and the unmodified photoanodes. Mechanisms should also be interpreted in conjunction with other data collected from the EIS, PL-quenching response and the J–V characteristic, not from one of these features alone. Any statistical variation that occurs between devices should be reported because it is important to be able to differentiate true changes in the device from changes due to the fabrication and measurement processes. Also, the ageing environment should be specified clearly so that it can be determined if changes are due to ageing or due to the combination of fabrication and measurement processes.

Where possible, operando measurements (or measurements performed in contact with the electrolyte) should be given more attention as the energetics of the interfaces could change during operation due to ion adsorption, solvent organization or electrolyte composition. But such an approach using computational and experimental methods is another avenue to the solution of these effects. The energy-level alignment of the dyes and TiO_2, charge-transfer dynamics, and dye anchoring configurations can be studied by DFT and TD-DFT calculations, while operando spectroscopy and electrochemical studies can be used to verify the energy-level alignment of the dyes and TiO_2, and the charge-transfer dynamics and anchoring configurations predicted in these calculations in the working DSSC. These synergies can offer a better foundation to establish a relationship between the modification of the TiO_2 and the dynamics of the charges at the interface and eventually in photovoltaic performance.

12.0 CONCLUSION

The literature reviewed within 2024-2026 further supports the main conclusion of this review: Optimizing the band structure along with the defects, morphology and interfacial chemistry in DSSCs is most fruitful when these three aspects are considered as one. The positive effect observed can be achieved by in-doping, Ti^{3+} engineer, Ag/Mg/Al/Ce doping, facet control, 1D/hierarchical architectures, carbon-based composites, heterostructures or passivation, but the positive effects are often coupled with more than one of these changes. These recent studies also discovered that overloading the dopant and/or composite can counteract the benefits and cause an increase in number of scattering centers, blocking of transport, reduction of dye-exposure, or introduction of recombination pathways.

Thus, another challenge in the research will be to ensure that the entire energy landscape is engineered at the molecular level and maintained with a high dye loading and at a low recombination position. The most promising future investigations will entail material verification, interface-sensitive energy measurements, and transient measurements of charge transfer, replicated photovoltaic data and stability testing. The benefit of an interfacial energy-level engineering can be considered as being independent of the optical absorption and/or surface structure degradation/defects added by the interfacial engineering.

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