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A Transfer Matrix Approach to Aid in The Design and Optimization of Hybrid Advanced Passive Structures for Enhancing Photovoltaic Efficiency

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Abstract

The addition of a luminescent down-shifting (LDS) layer directly onto a photovoltaic (PV) cell introduces additional loss mechanisms within the system. The combination of non-ideal photo-luminescent materials encapsulated within a limited range of viable host materials, with the increased reflection losses arising from the newly created interface represent losses which must be overcome for LDS to offer an enhancement to the underlying cells efficiency. Exploiting the interaction between the highly enhanced electric fields established close to a metal nanoparticles (MNP's) surface is one route aimed at mitigating the poor optical properties of the luminophore-host combinations available. Alternative approaches, aimed at addressing the other loss mechanisms within such a system have gone relatively unexplored. Exploiting the non-ideal nature of the photo-luminescent materials available, offers a possibility of recycling the photons which previously did not undergo photoluminescence while also addressing the reflection losses through the inclusion of selectively reflecting optical structures. The hybrid device designs, incorporating single- and double layer- antireflection coatings composed of commonly available materials offer enhancements in the underlying PV cells performance of 8% - 30% depending upon the design criteria established. The transfer matrix approach adopted allowed the impact of individual design considerations on the reflection suppression capabilities of the structure, as well as their impact on the underlying cells efficiency to be readily determined.

Keywords: Spectral losses, Photovoltaics, Photoluminescence, Plasmonics, Nanophotonic's, Optical modelling

1. Introduction

Using luminescent materials to capture high energy photons, previously poorly utilized by a cell, and re-emit the energy at a longer wavelength, where a cell is more efficient, led to the development of luminescent down-shifting (LDS) layers as a potential solution to increase the efficiencies achievable by PVs (Strümpel et al. 2007; Klampaftis et al. 2009; Thomas, Wedding, and Martin 2012; Ahmed et al. 2013; Ahmed, Doran, and McCormack 2016; Ahmed, McCormack, and Doran 2016; de la Mora et al. 2017). The enhancement offered by LDS is limited by the optical properties (low luminescent quantum yield, re-absorption losses, fluorescent quenching, etc.) of the luminescent and encapsulating materials (Klampaftis et al. 2009; Rothemund 2014; Ahmed, McCormack, and Doran 2016; Ahmed et al. 2013; de la Mora et al. 2017).

Further enhancements in the short wavelength response of PV technologies can be enabled by exploiting the plasmonic interaction between a specific combination of metal (e.g. Ag) nanoparticles (NPs) and luminescent species. The highly localized electromagnetic fields established on a nanostructures surface, tailored through the structures morphology and size, allow the optical properties of luminescent species within the near fields to be augmented. Enhancements in the optical properties of luminescent materials, previously deemed non-viable for their inclusion in an LDS device due to their poor optical characteristics, has showcased the merits of including nanostructures within the encapsulating material (Smitha et al. 2008; Shen et al. 2009; Power 2011; Chen et al. 2013; Ahmed, McCormack, and Doran 2017; Rothemund et al. 2011). The wide range of synthesis routes, structure morphologies, and material combinations possible allows the optimization of such plasmonic enhanced luminescent down shifting (PLDS) designs.

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The premise of using additional optical structures, which are selectively reflecting, would allow recycling the photons that did not previously interact with the luminescent species present within a PLDS layer. Increasing the probability of a photoluminescence event, mitigating some of the losses associated with the non-unity luminescent quantum yield of the luminophore, through the recycling of these photons. Exploiting the Stokes shift between absorption and emission peaks of a luminescent species pushes the boundaries of the enhancement attainable with a conventional PLDS approach. The optical structures consisting of a series of 'anti-reflection' type coatings would permit a high reflectivity of photons within a luminophores absorption range, a moderately low reflectivity across the remaining the response range being still present (Walshe et al. 2016).

The effect of the design of single- and double-layer reflecting structures, constructed using materials commonly used in the fabrication of antireflection coatings, on the performance of a mono-crystalline silicon (mc-Si) solar cell was theoretically evaluated. By adopting a transfer matrix approach, the effect of each design parameter was evaluated in terms of its impact on the underlying solar cells performance. The aim is to establish a set of initial design considerations that will allow for both the development of a prototype device and further refinement in the design of such devices. This can be achieved by employing the model developed i.e. using more complex structure designs, different luminescent species, different nanoparticle morphologies or a different underlying PV cell type.

2. Structure Enhanced Luminescent Down-Shifting (SE-LDS)

The addition of an LDS layer directly on top of a PV cell increases the number of loss mechanisms available within the system (Klampaftis et al. 2009; Rothemund 2014). The non-ideal optical properties of the luminescent materials available, coupled with losses introduced through the parasitic absorption and poor photo-stability of the encapsulating materials, will allow further design revisions (McKenna and Evans 2017; de la Mora et al. 2017; Mayr 2016; Klampaftis et al. 2009). The typically low refractive index (n = 1.5 – 2.2) of the host materials employed in LDS devices to date is introducing reflection losses from the LDS layers front surface (McKenna and Evans 2017). Structure-enhanced LDS (SE-LDS) devices (figure 1A) could be one such design option as it is allowing to recycle photons and, also, minimizing the surface reflection losses introduced through the addition of the LDS layer.

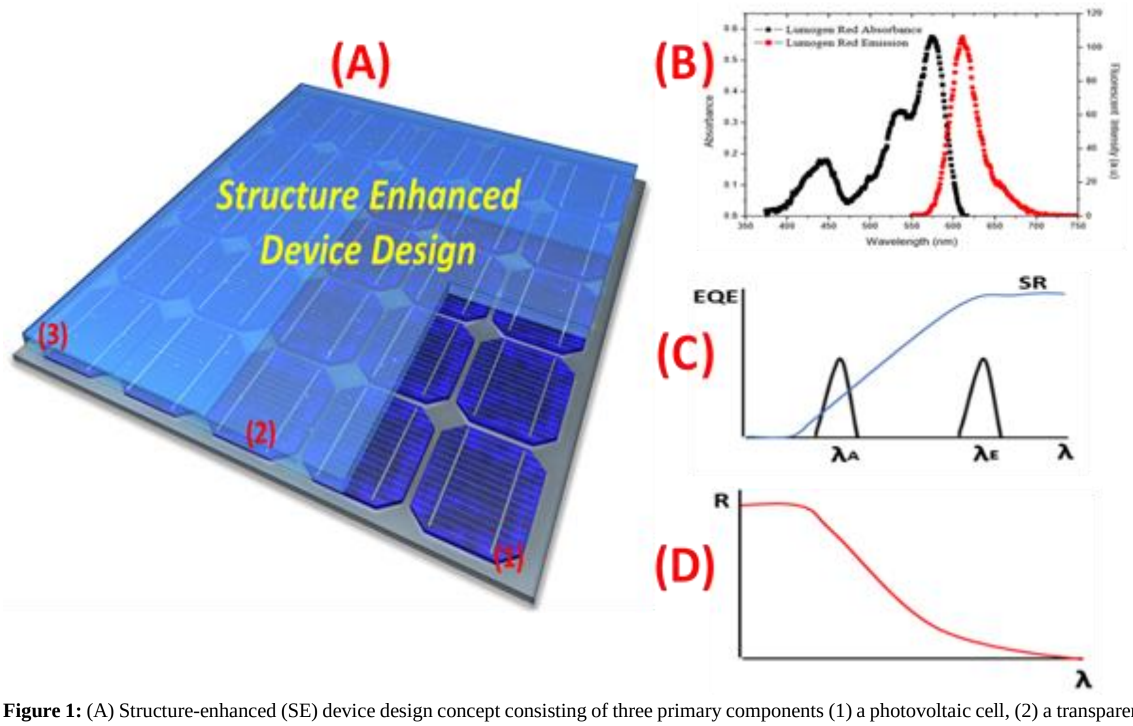

Figure 1: (A) Structure-enhanced (SE) device design concept consisting of three primary components (1) a photovoltaic cell, (2) a transparent matrix encapsulating either a luminescent material (B) or a combination of a luminescent material and metal nanoparticle and (3) a selectively reflecting coating with a reflection profile similar to that presented in (D). The selectivity of the reflecting structures can allows for recycling the photons lying within the encapsulated luminophore's absorption band (λ_A). This allows more photons to be shifted to higher wavelengths (λ_A) where the cells spectral response (SR) is greater (C)

The combination of a relatively small Stokes shift and the sub-unitary LQY are pushing for exploring more energy efficient architectures and novel design considerations. Through selectively designing the reflecting structures (similar to ARC's) a graded reflectivity profile (figure 1D) can be generated allowing for the recylcing of photons, which previously did not get a chance to undergo photoluminescence.

Utilising the formation of highly localized electromagnetic (EM) fields established within metal nanostructure vicinity further mitigates the loss mechanisms inherent within their electronic structure. Incorporating metal nanostructures within the transparent host media offers the capability of augmenting the luminophores optical properties through careful control of the nanostructures composition, morphology, physiochemical characteristics and size (Stalmashonak, Seifert, and Abdolvand 2013; Wiley et al. 2006; Ahmed, McCormack, and Doran 2017; Ahmed, Doran, and McCormack 2016; Zimbone et al. 2015; Power 2011; Smitha et al. 2008). Combining the PLDS approach with the structural enhanced element proposed here could allow for further enhancements in the cell performance.

3. Transfer Matrix Model

The propagation of light through a multi-layered structure, consisting of a series of thin dielectric media, with the variation between the refractive indices of subsequent layers varying significantly can be evaluated using a Transfer matrix model (TMM)(L, Matthew, and S 2007; Sánchez-Soto et al. 2012; Sahouane and Zerga 2014; Shabat and Ubeid 2014; Saylan et al. 2015; Shabat, El-Amassi, and Schaadt 2016; Sikder and Zaman 2016; Hamouche, Shabat, and Schaadt 2017). The TMM utilizes Maxwell's equations to connect the electric and magnetic field components across an existing boundary between two different isotropic dielectric media, allowing the interaction of the incident light with a single layer to be represented as a 2x2 transfer matrix (L, Matthew, and S 2007; Sánchez-Soto et al. 2012; Sahouane and Zerga 2014; Shabat and Ubeid 2014; Saylan et al. 2015; Shabat, El-Amassi, and Schaadt 2016; Sikder and Zaman 2016; Hamouche, Shabat, and Schaadt 2017). Extending this process to a multilayer structure is carried out through the determination of the matrix of each individual layer, with the overall systems matrix being the product of the individual layers matrices. The overall structures matrix is then converted back into transmission and reflection amplitude coefficients, allowing the resulting reflection, absorption and transmission spectra for complex multilayer structures to be readily determined.

4. Design Considerations

The wide range of ARC architectures, the different types of luminophore available and the tuneability of nanostructures granted by the numerous synthesis routes available allows for a large number of design considerations. To prove the viability of the SE-LDS concept only the simplest of structure designs were considered, consisting of single- and two-layer 'Bragg' structures. Here, the effect of the structures design and the numerous design parameters that are available were investigated using the transfer matrix approach. Two initial designs were selected for SE-LDS mc-Si devices (figure 2).

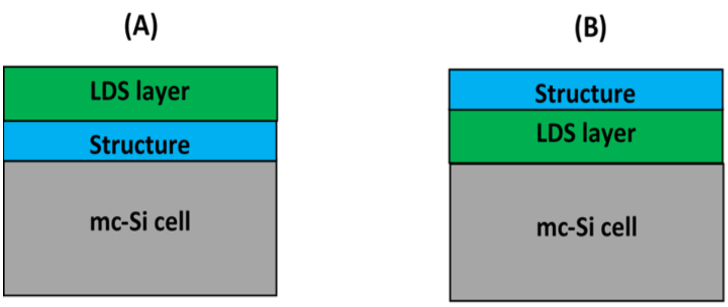

Figure 2: Initial designs for a structure-enhanced luminescent down-shifting (SE-LDS) mc-Si device with the selectively reflecting 'Bragg' structure situated (A) below the LDS layer and (B) above the LDS layer

Anti-reflection coatings (ARC's) can consist of a single layer or multilayer structure, with multilayer coatings offering the possibility of a greatly reduced broadband reflectance at one or more reflectance minima. Selectively reflecting structures were designed using both single and two layer ARC's to produce maximum reflection suppression at a series of wavelengths across the spectral range investigated (300nm – 1100nm), allowing the optimal materials and corresponding thicknesses to be determined for each structure investigated. Based upon the idealised refractive indices for both single and two layer ARC type structures, a range of suitable materials whose refractive indices lay both above and below the ideal values were considered. The materials utilized in the study outlined in table 1.

Table 1: List of the materials used to design structure enhanced elements (Green and Keevers 1995; Raut et al. 2011; 'SOPRA materials database' 2017; Polyanskiy 2017)

Single layer	Two layers
MgF_2	MgF_2-SiO
SiO	MgF_2-CeO_2
CeO_2	MgF_2-ZnS
ZnS	SiO_2-Si_3N_4
Ideal	MgF_2-Ta_2O_5
	MgF_2-TiO_2
	Ideal

To develop a deep understanding of the effect of the individual optical parameters (structure composition and design, dispersive media, optically thick layers, non-homogenous media etc.) of the system, the study was separated into components of increasing complexity. Adding each new element individually allowed monitoring the effect of the reflection suppression capabilities of an array of different structure enahcned (SE) designs and the impact of SE when are incorporated in the architecture of a silicon based device. Refining the optical properties of such structures can lead to viable structural and material configurations for the architectures of the SE-LDS (or PLDS) devices. As an initial approximation, all media are represented as being non-dispersive and homogeneous, with the optical properties of a layer being quantified by a single value of the refractive index and of the thickness.

5. Structure Enhanced (SE) Luminescent Down-Shifting (LDS) Devices

The single layer (SL) antireflection (AR) structures, comprising of the materials previously employed in two different design configurations, highlighted the ability of such simple structures to offer significant enhancements in the underlying cells performance (figure 3). Placing the AR structures below an LDS layer resulted in the greatest enhancement in device performance, with an 8% - 18% improvement in overall device achieved performance (figure 3A). The only instance in which a decrease in performance was observed was when the design included MgF_2. The MgF_2 refractive index is lower than the represented LDS layer, mitigating the π phase shift occurring when the $n1 < n2 < n3$ condition if fulfilled.

Through careful control of the AR structures composition and design, the enhancement factor can be maximised, with the maximum performance occurring for structures designed to suppress reflections at 600 nm - 650 nm. Reducing the thickness of the LDS had little effect on the enhancement offered by the addition of such structures to a LDS equipped device, leading to a 0.1% - 0.4% variation in the enhancement.

Considering the AR structure above an LDS layer resulted in a decrease in the overall device performance (figure 3B). As the light propagates from a media of lower refractive index to one with a higher index, it undergoes an 180^0 phase shift at the interface. This condition is only fulfilled for the structure design incorporating the material MgF_2 (figure 3B). Without the fulfilment of this condition the waves reflected from the two interfaces within such a system don't produce destructive interference but rather a collective of both constructive and destructive interference. The remaining materials employed possessed a refractive index larger than the polymer (PMMA) used to represent the LDS layer throughout the study. Decreasing the thickness of the LDS layer from 90 μm to 9 μm reduced the decrease in device performance for the majority of designs investigated (figure 3B) with values between 1% and 3%.

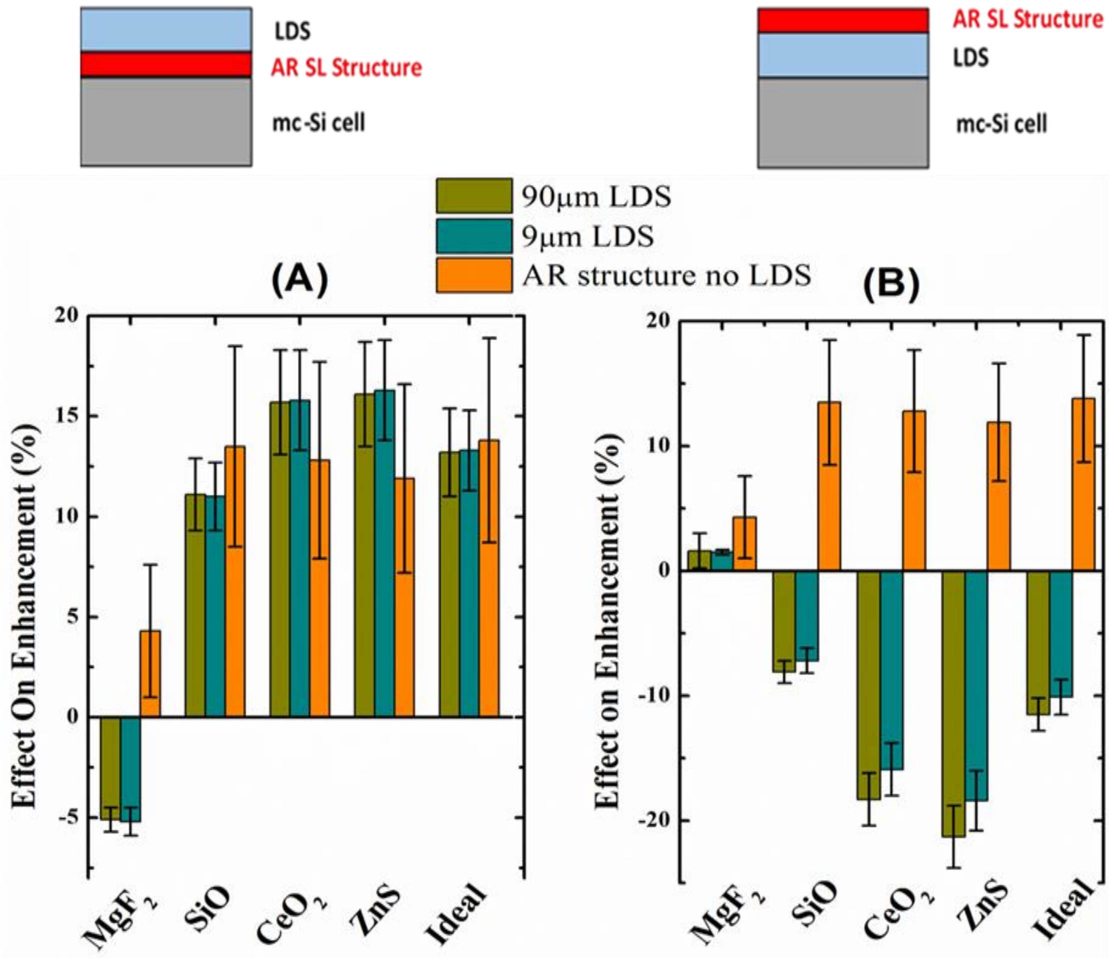

Figure 3: Average percentage (%) increase in the performance of mc-Si when fitted with two different structure enhanced LDS designs: (A)antireflection single-layer structure deposited directly below an LDS layer and (B) the antireflection single-layer structure deposited above. In all cases, the optical properties of the LDS layer were considered to be the optical properties of the polymer matrix material (PMMA), with two different layer thicknesses (90 µm and 9 µm). The variation in the levels of enhancement reported for each material is due to the variation in the wavelength at which the structures were designed to suppress reflection (λ0). Schematics of the design under consideration are included in the figure for each case.

Increasing to two the number of layers comprising the AR structure offered an even greater degree of enhancement in device performance (figure 4). The same trend for both initial outlined designs was reported. Placing the AR structure above the LDS layer results in a decrease in the mc-Si performance with values between 5% and 20% (figure 4). Initially, the SE devices designs that incorporated a selectively reflecting structure directly above the LDS layer (figure 3B and figure 4B) have shown no merit in enhancing the mc-Si cells performance and, consequently, they could be non-viable options.

Housing the AR structure between the LDS layer and mc-Si cell led to enhancements of 10% -24% in the cells energy conversion efficiency (figure 4A). Irrespective of the material combination employed in the device design, the cells performance was increased by 10% (figure 4). Fine-tuning of the design parameters facilitates enhancements on the order of 24%, a slight increase from the increase in performance being reported for single-layer structure designs (figure 3). Reducing the LDS layers thickness produces an increase in the enhancement offered by the structures in figure 24A with values between 2% - 4%.

Fabricating a SE device such that the AR component is located between the LDS layer and underlying PV cell shows the premise to deliver a significant enhancement to the PV cells conversion efficiency (figures 3A & 4A). In reality, the design process of the AR structures should contain a cost analysis element, whereby the advancement in the performance enhancement will need to be weighed against the cost of increasing the structures complexity.

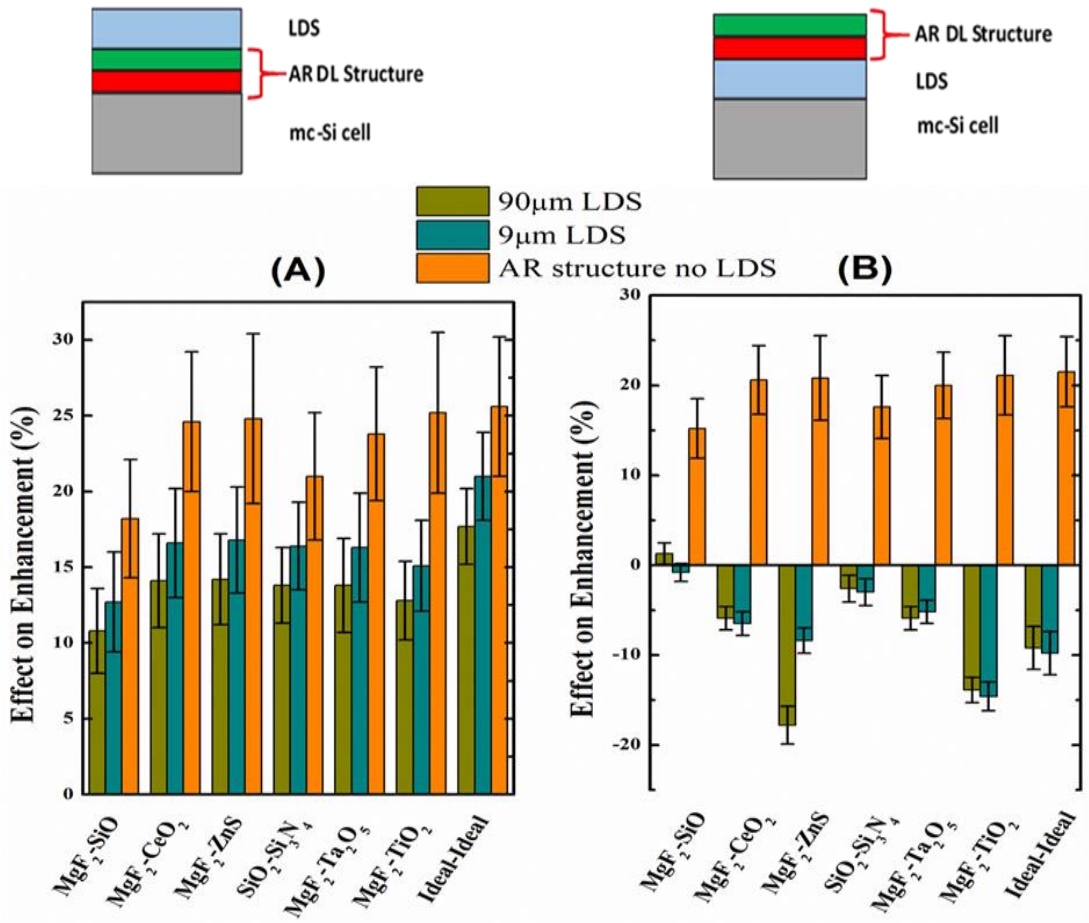

Figure 4: Average percentage (%) increase in the performance of mc-Si when fitted with two different structure-enhanced LDS designs: (A) antireflection bi-layer structure deposited directly below an LDS layer and (B) the antireflection bi-layer structure deposited above. The LDS layer in all cases have the optical properties of the commonly used polymer matrix material (PMMA) with two different layer thickness (90 μm and 9 μm). The variation in the levels of enhancement reported for each material is due to the variation in the wavelength at which the structures were designed to suppress reflection (λ_0). Schematics of the design under consideration are included in the figure for each case.

6. Conclusion

The premise of exploiting the incorporation of novel optical structures into the architecture of a mc-Si solar cell has been established using a TMM model. The structure designs considered highlighted their capacity to mitigate some of the loss mechanisms inherent in LDS and PLDS device designs. By careful selection of the design materials and the tolerance granted over their fabrication, the structures could offer potential device enhancements of 8% - 30% irrespective of photo-luminescent or metal nanostructure interactions. The transfer matrix approach adopted could potentially allow the design process to be automated and optimized for a given set of input criteria i.e. structure architecture, nanostructure and luminophore combination, as well as for the photovoltaic generation upon which the architecture is based. Refinements in the model investigated through experimental fabrication and characterization of such devices would help to establish a deeper understanding of the optical interactions within each component of the design.

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