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Aberrant effects on solar absorbance enhancement with the inclusion of dielectric coated plasmonic Cu-NP within hybrid organic-inorganic halide perovskite solar cell

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Research Article

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Abstract

In this paper we study the anomalous effects on solar absorbance with the insertion of dielectric coated plasmonic metal nanoparticle within hybrid organic-inorganic halide perovskite solar cell. It has been observed that the insertion of the metal@dielectric core-shell nanoparticles in the active layers of thin film organic solar cells enhance their conversion efficiency. The metal core increases the optical absorption, subsequently the conversion efficiency of thin film organic solar cells due to Localized surface plasmon resonance (LSPR) based field enhancement effect, the dielectric shell plays a key role to keep the metal core inaccessible so that it cannot offer recombination centre of the light-induced excitons. A comparative study conducted between the incorporated Au@SiO₂, Ag@SiO₂, and Cu@SiO₂, to validate the utilisation of coreshell copper nanoparticles for designing Perovskite solar cells (PSCs) with enhanced light trapping ability. The simulation results based on finite difference time domain shows the absorbance enhancement depends on the refractive index and the depth of the dielectric coating. The dielectric layer with high refractive index demonstrates the steady change in enhancement than the low refractive index dielectric layer with the variation in the depth of the shell. These unusual effects expand our knowledge on plasmonic PSCs and thus open the doors for its optimised design with enhanced light trapping ability. On comparison with different available core metals it is being observed that the copper@dielectric offers better chemical and thermal stability with increased absorption. It further lowers down the production costs of these designs, enabling them to be utilized even within the underdeveloped countries.

1. Introduction

With the escalating energy crises, Methylammonium lead halide (MAPbI₃) Perovskite solar cells (PSCs) have emerged as the considerable source of research interest due to their direct bandgap property, large material absorption coefficient, high carrier mobility, high efficiency, low temperature solution processability, high defect tolerance, long charge diffusion, mechanical flexibility, and simple preparation process [Petrović et al. 2015]. In recent years, they have also become commercially attractive owing to their low production costs. Over the past decade, power conversion efficiency (PCE) of the perovskite solar cells has remarkably increased from 3.8–25%. [J. Y. Kim et al. 2020]

Despite significant progress in its performance and power conversion efficiency (PCE), these hybrid organic-inorganic halide perovskite solar cells (PSCs) face serious challenges associated with their poor stability [M. Abd Mutalib et al., 2018]. Apart from the technical issues, lead toxicity is a vital environmental issue which poses a severe threat to its commercialization. To minimize the influence of a potential leak, the thickness of the perovskite film in this work is optimised to 200 nm, which is below than its set threshold of ~350nm. Recent analysis of these photovoltaic systems has also highlighted major concerns associated with their low absorption efficiency at longer wavelengths λ [600, 800] nm [S. Carretero-Palacios et al. 2015]. The light trapping ability of these cells can be drastically improved with the inclusion of metallic nanoparticles within the perovskite film of the PSCs. Plasmonics [Z. Zalevsky et al. 2014] can be defined as the interaction of incident light with the free conduction electrons of metallic

nanoparticles. Embedding metallic nanostructures within the thin perovskite films could serve as an effective strategy to significantly enhance the performance of PSCs, depending upon the virtue of its light driven characteristic property called localised surface plasmon resonance (LSPR). LSPR is an optical phenomenon arising due the collective oscillation of free conduction electrons at a particular frequency of incident light. The metallic nanostructures display LSPR towards the red part of the visible spectrum. The far and near field effect produced by nanoparticle (NP) embedded within the perovskite film leads to strong scattering, and enhanced electric field intensity in its surroundings, respectively. Ultra-thin high efficiency solar cells are also designed based on the near field effect produced by these nanoparticles. Variation of shape, size and the concentration of the nanostructures influences the peak position and intensity of the localised surface plasmon resonance, thus affecting the absorption efficiency of PSCs [Sahai et al. 2021 OQE, Sahai et al. 2021].

On the basis of previous work, we focus on embedded plasmonic nanoparticles in organic, perovskite solar cells. We then study models for embedded coreshell plasmonic nanostructures in photovoltaic thin films and evaluate the model in the perspective of previous results in the field. To yield more photocurrent within the methylammonium lead iodide-based devices, embedded metallic nanoparticles in PSCs are coated with a dielectric shell [C. Shen et al. 2014]. Previously conducted research showed that we can use various dielectric materials like SiO₂, TiO₂, Al₂O₃, ZnO etc on the basis of their stability and availability. The thickness of dielectric plays a vital role in providing thermal and chemical stability of metallic NPs. Further, dielectric coating prohibits metallic NPs from acting as charge recombination centers. Recent studies indicate that the dielectric coating results in a reduction of light harvesting ability of these cells as compared to the absorption efficiency produced by bare metallic nanoparticle. In addition, utilisation of plasmonics within the perovskite solar cells also promote carrier mobility, electron transfer and exciton dissociation. LSPR is also utilised for different applications, varying from optical communication to photovoltaics. Thickness of the coating may vary from 1 to tens of nanometres.

Previous study done by Zhang [Zhang et al. 2013] highlights enhancement in the photocurrent and reduction in absorption ability of the designed solar cell with the incorporation of the coreshell Au@SiO₂ nanoparticle. The device achieves an efficiency of 11.4% [Zhang et al. 2013]. Further, the work done by Saliba [Saliba et al. 2015] suggests the impact of incorporating temperature sensitive coreshell Ag@TiO₂ nanostructures within low temperature processed solar cells, and thus boosting its efficiency to 16.3% [Saliba et al. 2015]. In the work by Dabirian [Dabirian et al. 2016], the inclusion of monolayer of coreshell Silica@Ag nanoparticles within the dye sensitized solar cells, leads to a significant improvement of 38% in its short current density [Dabirian et al. 2016]. The study carried on by Carretero-Palacios [Carretero et al. 2016] indicates the impact of embedding different shapes, materials, and sizes of the plasmonic metal nanoparticles within the solar cell. It has been observed that silver nanoparticles provide the largest enhancement compared to other metallic nanoparticles. It further explains that the amount of light absorbed by the nanoparticle depends upon the depth at which it is embedded. Pathak [Pathak et al. 2017] experimentally verifies the potential of incorporating core-shell Au@SiO₂ nanoparticles, and thus leading to enhanced photocurrent for the plasmonic solar cell. The device achieves an efficiency of 18%

[Pathak et al. 2017]. J. Cui reports the impact of embedding spectrally tuned $Au@SiO_2$ nanospheres and nanorods into the inverted perovskite solar cells with a power conversion efficiency of 13.7% [Cui et al. 2016]. A significant increase in the photocurrent of the device could be attributed to the LSPR in the infrared region of the electromagnetic spectrum.

Luo [Luo et al. 2017a] combined Au nanoparticles with MgO passive layer. Introduction of a passive layer of MgO enhances the short circuit current and solar absorption of the device and provides further stability to the designed PSCs under the UV light. An increase in the electrostatic potential of the device is also observed with the incorporation of Au@SiO₂ nanostars into the mesoporous layer of TiO₂ and thus achieving an efficiency of 17.72% [Batmunkh et al. 2017]. Improved efficiency of 20.1% is attained with the inclusion of Au@TiO₂ into the TiO₂ layer of PSCs [Fan et al. 2017]. A theoretical study by Heidarzadeh reports a significant enhancement in the performance of PSCs with the introduction of core-shell Au@SiO₂ dimer nanoparticles [Heidarzadeh 2018]. A recent study conducted by C. Shen [C. Shen et al. 2014] explores the impact of embedding coreshell nanoparticles with varying refractive index of the dielectric coating.

All the studies carried out in the past to enhance the performance of PSCs with the introduction of coreshell are done using expensive metallic NPs eg silver or gold. These Nanoparticles are definitely stable and provide very good results but we must explore some low cost yet effective substitutes of nanoparticles. Our previous work suggests that copper nanoparticles [Sahai et al. 2021, Sahai et al. 2021 OQE] serve as a cheaper alternative to gold and silver nanoparticles without compromising the light trapping ability of PSCs. On the basis of the inference of our previous study in this paper we present a detailed theoretical study to elucidate the impact of coreshell Copper nanoparticles with different dielectric coatings like SiO₂ and TiO₂. A comparative study based on finite difference time domain method, has been conducted to analyse the influence of dielectric coating of high and low refractive index on the copper nanoparticle in the yielding of photocurrent of PSC. The results depict that the absorption reduces as we increase the thickness of the dielectric coating, keeping the fill factor constant. We may also infer from the results that the rate of reduction of absorption is higher for low index dielectric covering. It has been observed that PSC with coreshell nanoparticle capitulate photocurrent 30.2194 mA/cm² for Cu@SiO₂ and 30.6062 mA/cm² for Cu@TiO₂, keeping the Cu core radius 69 nm and shell of 1nm thick. These unusual effects expand our knowledge on plasmonic PSCs and thus laying guidelines for its optimised design with enhanced light trapping ability.

2. Simulation Setup

For the calculation of optical properties, the three-dimensional Finite Difference Time Domain method of simulation is employed. Inclusion of a coreshell Copper nanoparticale (Cu-NP) significantly enhances the absorption efficiency of the designed solar cell with the volume of $L_X X L_Y X L_Z$ for a unit cell. Figure 1 shows the schematic model of PSCs embedded with a plasmonic copper nanoparticle. Here the Copper nanoparticle is coated with a dielectric material. Earlier the research was carried out using various

dielectric materials like SiO2, Al₂O₃, ZnO, TiO₂. Where, SiO₂ has minimum refractive index while TiO₂ has the maximum refractive index among these therefore we choose these two dielectrics to investigate the performance of the designed cell. Figure 1 inset portrays a coreshell copper nanoparticle of total radius r nm, with the altering thickness of shell d nm. To curtail the risk of lead toxicity, the thickness of the perovskite film is further optimised to 200 nm. Spiro-OMeTADacts as a hole transport material, which not only provides stability to the designed solar cell but also leads to an enhancement in its performance. The thickness of the semi-infinite glass layer, acting as a substrate is set to 100 nm. The real and imaginary part of the refractive index of perovskite (CH₃NH₃Pbl₃) layer are represented by $n_p(\omega) = n(\omega) + ik(\omega)$. This data is extracted from the experimental values given in [Filipič et al. 2015, Johnson et al. 1972, Zhang et al 2015]. Figure 2 depicts the plot of its real and imaginary values as a function of wavelength. It further leads to the conclusion that the wavelength range of perovskite is according to its imaginary part of the refractive index. Note, a small variation in the optical constants of the metal and perovskite materials have a significant impact on the performance of PSCs. The refractive index of the spiro-OMeTAD (n_s) and the glass substrate (n_g) are taken as 1.7 and 1.5, respectively. E D Palik [Palik 1985] reports the refractive index of copper nanoparticles. Representatively, the chosen dielectric shell materials, SiO_2 and TiO_2 have a refractive index of 1.45 and 2.61 over the visible region. [Palik 1985, Deng et al. 2019]

The designed perovskite solar cell is irradiated with a plane wave as shown in Fig. 1, propagating along the *z* direction whose intensity is normalised to match the standard solar power spectrum. Periodic boundary conditions are applied in the *x* and *y* direction while a perfectly matched layer (PML) is applied in the *z* direction to prevent further optical losses. A high mesh density of 5 nm is applied to achieve elevated accuracy and convergence of results. The total absorption [Omelyanovich et al. 2016,Ghahremanirad et al. 2017,Ghahremanirad et al. 2018] of the designed perovskite based solar cell is calculated by (Eq. 1)

$$P_{abs} = \int \varepsilon_o \omega(\lambda) |E(x, y, z, \lambda)|^2 n(\lambda) k(\lambda) dV$$
⁽¹⁾

Here ω is defined as the angular frequency, E is the electric field, Vis the volume and λ is the wavelength of light

Ideal short circuit current is considered to examine the light trapping ability of each nanostructure. J_{SC} calculated from the solar generation package gives the electron-hole pair obtained by light absorption of the device. It does give the actual short circuit current from the designed solar cell but reflects upon its light harvesting property. The total absorption enhancement in the cell is calculated by (Eq. 2) [Rahman et al. 2019]

$$Enhancement = \frac{J_{SC, withNP}}{J_{SC, withoutNP}}$$

Where $J_{SC, withNP}$ and $J_{SC, withoutNP}$ are the light absorption with the presence and absence of the nanoparticle (NP) within the PSC.

3. Theoretical Background And Study

Mie theory is explored to analyse the optical properties of dielectric coated and non-coated nanoparticles [Qiang et al. 2001,Wriedt et al. 2012]. This background study is trivial as lays the foundation of understanding how the presence of these nanoparticles within the PSCs influence its absorption efficiency. Mie theory gives the analytical solution of Maxwell's equations as the incident light is scattered by the particle of any size [Bohren et al. 1998]. This theory is confined to spherical nanoparticles but can be modified for other shapes [Bohren et al. 1998]. According to this theory absorption cross section $C_{absorption}$ can be defined as the difference between the extinction cross section $C_{extinction}$ and scattering cross section $C_{scattering}$ given by Eq. (3)

$$C_{absorption} = C_{scattering} - C_{extinction}$$

3

The calculated extinction cross section and scattering cross section is given by Eq. (4) and Eq. (5) respectively,

$$C_{extinction} = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} (2n+1) \operatorname{Re}\{a_n + b_n\}$$

4

$$C_{scattering} = \frac{2\pi}{k^2} \sum_{n=1}^{\infty} (2n+1)(|a_n|^2 + |b_n|^2)$$

5

In these set of equations, a_n and b_n are the scattering coefficients. k is defined as the wave number given by $k = 2Nn/\lambda$ where N is the refractive index of the medium in which the particle is embedded.

The scattering coefficients a_n and b_n are given by Eq. (6) and Eq. (7) respectively,

$$a_{n} = \frac{m\psi_{n}(mx)\psi_{n}(x) - \psi_{n}(x)\psi_{n}(mx)}{m\psi_{n}(mx)\xi_{n}(x) - \xi_{n}(x)\psi_{n}(mx)}$$

6

$$b_{n} = \frac{\psi_{n}(mx)\psi_{n}(x) - m\psi_{n}(x)\psi_{n}(mx)}{\psi_{n}(mx)\xi_{n}(x) - m\xi_{n}(mx)\psi_{n}(mx)}$$

In these equations, *m* is the relative refractive index, *x* is defined as the size parameter and is given x = kr where *r* is the radius of the particle. ψ_n and ξ_n are the Bessel functions.

The extinction efficiency is calculated by normalising the extinction cross section over the cross section of the nanoparticle [Du et al. 2004]. The amount of light adsorbed and scattered by the particle helps to determine the light harvesting ability of PSCs embedded with nanostructures over a particular wavelength range.

4. Results And Discussion

We have conducted a comparative study between different coreshell nanoparticles such as $Au@SiO_2$, $Ag@SiO_2$, and $Cu@SiO_2$ embedded within the solar cell. We have also thoroughly examined the impact of embedding coreshell nanoparticles with dielectric coatings SiO_2 and TiO_2 within the PSCs. These dielectrics are good photocatalysts and their coatings not only provide chemical stability to these particles but also thermal stability at high temperatures. They prevent the particles to act as charge recombination centers. The thickness of its dielectric shell is further investigated to optimise the design of our modelled PSCs.

4.1 Material of the core

The existing designs employ conventional metals such as coreshell gold and silver-based nanostructures within the perovskite solar cells. The inclusion of such plasmonic nanostructures within the PSCs significantly elevates its production costs and thus causes a severe threat to its commercialization. Our previous work [Sahai et al. 2021,Sahai et al. 2021] suggests that a copper nanoparticle of 70 nm radius embedded within a perovskite film of thickness 200 nm produces maximum absorbance, hence for this study the size of the core is fixed at 69 nm, while the thickness of the shell is 1nm. The particle is placed at the centre of the film. Figure 2 reveals solar absorbance enhancement with the incorporation of different coreshell nanoparticles such as Au@SiO₂, Ag@SiO₂, and Cu@SiO₂ within perovskite film. We observe that a Cu@SiO₂ produces similar absorbance as Au@SiO₂ and Ag@SiO₂. The inset clearly depicts that the absorbance wavelength for Cu@SiO₂ is red shifted towards the longer wavelength as compared to Ag@SiO₂. We also calculate the enhancement factor for these particles from Eq. 2. The J_{SC} calculated for perovskite films without a nanoparticle is 17.8421 mA/cm² whereas with a cu nanoparticle it shows 31.165 mA/cm². Further we get maximum enhancement of 1.693 for Cu@SiO₂, thus making it a potential candidate for designing PSCs with low-cost and high stability.

Table 1 Calculation of the J_{SC} and the enhancement factor for different core nanoparticles with shell as SiO₂

Material of the core	J _{SC}	Enhancement	
	mA/cm ²		
Ag	26.568	1.489	
Au	27.944	1.566	
Cu	30.219	1.693	

4.2 Material of the shell and its thickness

In our previous study [Sahai et al 2021,Sahai et al. 2021] we found that due to the double contribution of near and far field effects, a spherical copper nanoparticle of 70 nm radius, placed at the centre of the 200 nm thin perovskite film produces maximum absorbance, hence we further extend our work by varying the thickness of the core and the shell, keeping the fill factor constant at 70%. It is placed at equal distances from both Spiro-OMeTAD and glass substrate.

Figure 3 describes the absorbance spectra for nanoparticles with dielectric shells SiO_2/TiO_2 , i.e., $Cu@SiO_2$ [Varshney A. et al. 2022] and $Cu@TiO_2$. The nanostructure without any shell implicates when d = 0 nm acts as a reference to investigate the enhancement in the light trapping ability of the coreshell nanoparticles embedded within the perovskite film. It produces an absorbance spectrum within the visible range ($\lambda > 600$ nm).

When the dielectric shell is introduced, its refractive index plays a key role in determining the enhancement in its absorbance efficiency. Figure 3 (a) and (b) portray the extinction spectrum of nanostructures placed in perovskite medium, with different thickness of core and shell thus keeping the total size of the particle constant at 70 nm. Interestingly, we observe that with the increase in the shell thickness from d = 0 nm to d = 15 nm, and a simultaneous decrease in the size of the core from r = 70 nm to r = 55 nm respectively, the extinction efficiency decreases sharply for Cu@SiO₂ as compared to Cu@TiO₂. The results portrayed by Fig. 3 (c) and (d) further justify the above argument, as the absorbance intensity of Cu@SiO₂ decreases sharply with the enhancement of the shell thickness, while a gradual decrease in the absorbance ability of Cu@TiO₂, along with slight red shift in its wavelength range.

Table 2 shows the J_{sc} of these coreshell nanostructures. It is utilised to examine the absorption efficiency of these cells. The J_{sc} for PSCs without any nanoparticle is found 17.8421 mA/cm². The enhancement factor is calculated according to the Eq. 2. Figure 4 clearly conducts a comparison between the enhancement ability of the designed PSC with the change in the thickness of its shell. A sharp reduction

in the enhancement factor is observed for $Cu@SiO_2$ as compared to $Cu@TiO_2$, embedded within the perovskite film.

Table 2: Calculation of the J_{SC} and enhancement factor with the insertion of different Cu@dielectriccoreshell nanoparticles within thin perovskite film of PSCs

Size of the core (nm)	Size of the shell (nm)	Material of the shell			
		SiO ₂		TiO ₂	
		J_{SC}	Enhancement	J_{SC}	Enhancement
		mA/cm ²		mA/cm ²	
70nm	0nm	31.0071	1.7378	31.0071	1.7378
69nm	1nm	30.219	1.6937	30.6062	1.7153
68nm	2nm	29.699	1.6645	30.3393	1.7004
65nm	5nm	26.088	1.4621	28.7349	1.6105
60nm	10nm	23.816	1.3348	27.5722	1.5453
55nm	15nm	21.737	1.2182	25.8843	1.4507

The electric field intensity is governed by the boundary conditions at the interface of the particle. We note that the electric field intensity of the particle coated with a material of higher refractive index enhances significantly as compared to the particle with lower refractive index. Figure 5 (a) represents the electric field intensity of $Cu@SiO_2$ with a core of 69 nm and a shell of 1nm. As the thickness of the shell increases to 15 nm, the electric field intensity as shown in Fig. 5 (c) decreases significantly. Note, the electric field decreases exponentially as we move away from the particle interface.

In addition, the dielectric shell of 1nm further provides chemical stability to the particle embedded within the perovskite film. The shell prevents the oxidation of the copper nanoparticles and thus helps maintain the efficiency of these devices for a longer duration of time.

Conclusion

In summary, we study the anomalous effects on solar absorbance enhancement with the insertion of dielectric coated plasmonic Cu-np within hybrid organic-inorganic halide perovskite solar cell. The insertion of the metal@dielectric core-shell nanoparticles in the active layers of thin film organic solar cells effects their conversion efficiency. It has been revealed that the metal core increases the optical absorption, and consequently the conversion efficiency of thin film organic solar cells due to LSPR based field enhancement effect, and meanwhile the dielectric shell avoids the metal core to offer recombination centre of the light-induced excitons.

The simulation results show the absorbance spectra and electric field intensity produced by particles with dielectric coating of lower refractive index increases significantly as the shell width shrinks. These aberrant effects expand our knowledge on plasmonic PSCs and thus open the doors for its optimised design with enhanced light trapping ability. On comparison with different available core metals eg. Au, Ag and Cu, it is being observed that the copper@dielectric offers chemical and thermal stability with increased absorption. It further lowers down the production costs of these designs, enabling them to be utilized even within the underdeveloped countries.

Declarations

Ethics approval: Authors of this manuscript have followed all the Ethical Responsibilities as per guideline of the journal

Consent to participate: Consent has been given as per journal policy.

Consent for publication: Consent has been given as per journal policy.

Availability of data and materials: This research work is based on FDTD simulations and all related material has been cited in reference session.

Competing interests: The authors have no conflicts of interest to disclose.

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Authors' contributions: 1. Shreya Sahai proposed the conception/design of the work. She did the data analysis and interpretation. She has drafted the article.

2. Anshu Varshney has given the conceptual direction and inspiration for the work. She revised the manuscript critically and gave her final permission before it could be published.

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References

- M. Petrović, V. Chellappan, and S. Ramakrishna, "Perovskites: Solar cells & engineering applications

 materials and device developments," Solar Energy, vol. 122, pp. 678–699, Dec. 2015, doi: 10.1016/j.solener.2015.09.041.
- 2. J. Y. Kim, J.-W. Lee, H. S. Jung, H. Shin, and N.-G. Park, "High-Efficiency Perovskite Solar Cells," Chem. Rev., vol. 120, no. 15, pp. 7867–7918, Aug. 2020, doi: 10.1021/acs.chemrev.0c00107.
- 3. M. Abd Mutalib et al., "Progress towards highly stable and lead-free perovskite solar cells," Mater Renew Sustain Energy, vol. 7, no. 2, p. 7, Mar. 2018, doi: 10.1007/s40243-018-0113-0.

- S. Carretero-Palacios, M. E. Calvo, and H. Míguez, "Absorption Enhancement in Organic–Inorganic Halide Perovskite Films with Embedded Plasmonic Gold Nanoparticles," J. Phys. Chem. C, vol. 119, no. 32, pp. 18635–18640, Aug. 2015, doi: 10.1021/acs.jpcc.5b06473.
- 5. Z. Zalevsky and I. Abdulhalim, "Chapter 6 Plasmonics," in Integrated Nanophotonic Devices (Second Edition), Z. Zalevsky and I. Abdulhalim, Eds. Oxford: William Andrew Publishing, 2014, pp. 179–245. doi: 10.1016/B978-0-323-22862-6.00006-2.
- C. Shen, L. Deng, N. Wang, and Y. Huang, "Anomalous effects of dielectric coated plasmonic metal nanoparticles on solar absorption enhancement in perovskite thin films," J. Phys. D: Appl. Phys., vol. 54, no. 30, p. 305501, May 2021, doi: 10.1088/1361-6463/abfe36.
- Zhang, W., Saliba, M., Stranks, S.D., Sun, Y., Shi, X., Wiesner, U., Snaith, H.J.: Enhancement of perovskite-based solar cells employing core-shell metal nanoparticles. Nano Lett. 13, 4505–4510 (2013)
- Saliba, M., Zhang, W., Burlakov, V.M., Stranks, S.D., Sun, Y., Ball, J.M., Johnston, M.B., Goriely, A., Wiesner, U., Snaith, H.J.: Plasmonic-induced photon recycling in metal halide perovskite solar cells. Adv. Funct. Mater. 25, 5038–5046 (2015)
- Dabirian, A., Byranvand, M.M., Naqavi, A., Kharat, A.N., Taghavinia, N.: Self- assembled monolayer of wavelength-scale core-shell particles for low-loss plasmonic and broadband light trapping in solar cells. ACS Appl. Mater. Interfaces 8, 247–255 (2016)
- 10. Carretero-Palacios, S., Jiménez-Solano, A., Míguez, H.: Plasmonic nanoparticles as light-harvesting enhancers in perovskite solar cells: a user's guide. ACS Energy Lett. 1, 323–331 (2016)
- 11. Pathak, N.K., Chander, N., Komarala, V.K., et al.: Plasmonic Perovskite Solar Cells Utilizing Au@SiO2 Core-Shell Nanoparticles. Plasmonics 12, 237–244 (2017)
- 12. Cui, J., Chen, C., Han, J., Cao, K., Zhang, W., Shen, Y., Wang, M.: Surface plasmon resonance effect in inverted perovskite solar cells. Adv. Sci. 3, 1–8 (2016)
- 13. Luo, A.Z.Q., Shi, J., Yue, L., Wang, Z., Chen, X., Huang, S.: Efficient perovskite solar cells by combination use of Au nanoparticles and insulating metal oxide. Nanoscale. 9, 2852–2864 (2017a)
- Batmunkh, M., Macdonald, T.J., Peveler, W.J., Bati, A.S.R., Carmalt, C.J., Parkin, I.P., Shapter, J.G.: Plasmonic gold nanostars incorporated into high-efficiency perovskite solar cells. ChemSus Chem. 10, 3750–3753 (2017).
- 15. Fan, R., Wang, L., Chen, Y., Zheng, G., Li, L., Li, Z., Zhou, H.: Tailored Au@TiO2 nanostructures for the plasmonic effect in planar perovskite solar cells. J. Mater. Chem. A. 5, 12034–12042 (2017)
- 16. H. Heidarzadeh, "Comprehensive investigation of core-shell dimer nanoparticles size, distance and thicknesses on performance of a hybrid organic-inorganic halide perovskite solar cell," Mater. Res. Express, vol. 5, no. 3, p. 036208, Mar. 2018, doi: 10.1088/2053-1591/aab6f3.
- 17. S. Sahai and A. Varshney, "Solar absorbance enhancement in perovskite solar cells with the inclusion of copper nanoparticles: an architectural study," Opt Quant Electron, vol. 53, no. 2, p. 111, Feb. 2021, doi: 10.1007/s11082-021-02755-9.

- S. Sahai and A. Varshney, "The Effect of Morphologies of Embedded Plasmonic Cu-nanoparticles on Solar Absorption of Perovskite Solar Cells: A Comprehensive Study," Optics and Spectroscopy, Volume 129, Issue 10, p.1165-1172, October 2021, doi: 10.21883/OS.2021.08.51206.1008-21.
- 19. Filipič, M., Löper, P., Niesen, B., de Wolf, S., Krč, J., Ballif, C., Topič, M.: CH3NH3PbI3 perovskite/silicon tandem solar cells: characterization based optical simulations. Opt. Exp. 23, A263–A278 (2015)
- 20. Johnson, P.B., Christy, R.W.: Optical constants of the noble metals. Phys. Rev. B 6(12), 4370–4379 (1972)
- 21. Zhang, W., Anaya, M., Lozano, G., Calvo, M.E., Johnston, M.B., Míguez, H., Snaith, H.J., "Highly efficient perovskite solarcells with tunable structural color," Nano Lett. 15, 1698–1702 (2015)
- 22. Palik E D 1985 Handbook of Optical Constants of Solid (New York: Academic)
- 23. Deng L, Zhai Y, Chen Y, Wang N and Huang Y 2019 Enhancing the plasmonic fields by high refractive index dielectric coating for surface enhanced spectroscopies J. Phys. D: Appl. Phys. 52 43LT01.
- 24. Omelyanovich, M., Makarov, S., Milichko, V., Simovski, C.: Enhancement of perovskite solar cells by plasmonic nanoparticles. Mater. Sci. Appl. 7, 836–847 (2016)
- Ghahremanirad, E., Bou, A., Olyaee, S., Bisquert, J.: Inductive loop in the impedance response of perovskite solar cells explained by surface polarization model. J. Phys. Chem. Lett. 8, 1402–1406 (2017)
- 26. Ghahremanirad, E., Olyaee, S., Nejand, B.A., Ahmadi, V., Abedi, K.: Hexagonal array of mesoscopic HTM-based perovskite solar cell with embedded plasmonic nanoparticles. Phys. Status Solidi B 255, 1–8 (2018)
- Md. S. Rahman, M. Ibrahim, S. Munira, and K. Pau, "Plasmon Enhanced Semitransparent Planar Perovskite Solar Cells with Copper Nanocubes: FDTD Study," in 2019 IEEE PES Asia-Pacific Power and Energy Engineering Conference (APPEEC), Dec. 2019, pp. 1–6. doi: 10.1109/APPEEC45492.2019.8994423.
- 28. Qiang, Fu., Sun, W.: Mie theory for light scattering by a spherical particle in an absorbing medium. Appl. Opt. 40, 1354–1361 (2001)
- 29. Wriedt, T.: Mie theory: a review. In: Hergert, W., Wriedt, T. (eds.) The Mie. Theory Springer Series in Optical Sciences, vol. 169. Springer, Berlin Heidelberg (2012)
- Bohren, C. F., & Huffman, D. R., "Absorption and Scattering of Light by Small Particles", Chapter 4 "Absorption and Scattering by a Sphere," John Wiley & Sons, Ltd, 1998, pp. 82–129. doi: 10.1002/9783527618156.ch4.
- Bohren, C. F., & Huffman, D. R., "Absorption and Scattering of Light by Small Particles", Chapter 3 "Absorption and Scattering by an Arbitrary Particle," Wiley & Sons, Ltd, 1998, pp. 57–81. doi: 10.1002/9783527618156.ch3.
- 32. H. Du, "Mie-scattering calculation," Appl. Opt., AO, vol. 43, no. 9, pp. 1951–1956, Mar. 2004, doi: 10.1364/AO.43.001951.

33. Varshney, A., Sahai, S. (2022). Nanomaterials' Architectural Study in Perovskite Solar Cells. In: Katiyar, J.K., Panwar, V., Ahlawat, N. (eds) Nanomaterials for Advanced Technologies. Springer, Singapore. https://doi.org/10.1007/978-981-19-1384-6_4

Figures



Figure 1

The schematic model of PSCs embedded with a plasmonic copper nanoparticle. The inset shows Coreshell copper nanoparticle with the core radius *r* nm and the depth of the shell *d* nm.



Solar absorbance enhancement with $Au@SiO_2$, $Ag@SiO_2$, and $Cu@SiO_2$ nanoparticles within the perovskite film. The inset depicts that the $Cu@SiO_2$ (yellow) shows similar absorbance as $Au@SiO_2$ (blue) and $Ag@SiO_2$ (red).



(a) Extinction efficiency of $Cu@SiO_2$ (b) Extinction efficiency of $Cu@TiO_2$ (c) Absorbance produced by $Cu@SiO_2$ within the perovskite film. (d) Absorbance produced by $Cu@TiO_2$ within the perovskite film. The thickness of the core and shell are varied from 70nm to 55nm and 0 to 15nm respectively.



Total enhancement in the light trapping ability of PSCs as a function of the shell thickness.



Electric field intensity (a) $Cu@SiO_2$ with d = 1 nm, r = 69 nm (b) $Cu@TiO_2$ with d = 1nm, r = 69 nm (c) $Cu@SiO_2$ with d = 15 nm, r = 55 nm (d) $Cu@TiO_2$ with d = 15 nm, r = 55 nm.