



Metasurface absorber based single junction thin film solar cell exceeding 30% efficiency

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Abstract: In this article, we report, as per our knowledge, for the first time, a thin film single junction solar cell with a metasurface absorber layer directly incorporated. We have used an interconnected dual inverted split ring resonator pattern in the InAsP absorber layer. The structure eliminated patterns of conventional metals, such as silver, aluminum, and gold, from the active layer, a common drawback in conventional solar absorbers, hindering their direct integration into solar cells. Optical simulation results show a peak ideal short circuit current density of 76.23mA/cm^2 for the meta-absorber structure under solar illumination. This current is the highest among previously reported absorbers based on Group IV materials and III-V compounds, overcoming the low solar absorption of such metasurfaces. The final proposed solar cell structure combines this meta-absorber layer with traditional efficiency enhancement methods namely anti-reflecting coating, textured back reflector, and transparent top electrode. This novel single junction structure shows a solar absorption efficiency of 97.86% and a power conversion efficiency of 30.87%, the highest for III-V solar cells. Our device proves the ability of metasurface absorber layers to produce high-efficiency solar cells and is expected to pave the way for integrating novel meta-devices into state-of-the-art photovoltaic devices, aiding the global transition towards clean energy sources.

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1. Introduction

Recent years have seen a significant shift towards renewable and non-conventional energy sources around the globe amid the growing concerns over climate change and depleting fossil fuel supply. Solar photovoltaic (PV) systems have been the front runner in this energy transition as the fastest-growing renewable energy source [1]. To meet the ever-increasing global energy demand in a safe, sustainable, and environment-friendly way, there has been a significant interest in the enhancement of the electrical and cost efficiency of solar cells over the last decade.

Thin film variant of solar cells has emerged as a cost-effective pathway for solar energy harvesting due to the use of less semiconducting material [2]. Apart from the traditional silicon-based structures [3,4], III-V [5–9] and perovskite (PVK) [10,11] compounds have also been heavily investigated as the active material of thin film solar cells (TFSC). The thin absorbing layer used in TFSCs decreases the photon absorption in the active region, degrading the overall efficiency of the device. This problem can be alleviated by increasing light transmission into the PV cell or absorption in the absorber layer. Several efficiency enhancement methods namely textured front surface for enhanced light in-coupling [12] and series resistance reduction [13], anti-reflective coating [14], transparent conducting electrode [15], patterned back reflector [16,17], nanowires (NW) [5], scattering and absorbing nanoparticles [18,19], quantum dots [9] have been used in previous works.

Metasurfaces have gained significant interest from the photonics research community for their ability to induce enhanced light-matter interaction. This distinct feature of these structures has also been utilized as light focusing element [20,21] and more commonly as broadband solar absorber [22–30] for solar energy harvesting in previous literature. The nanoscale metallic

patterns and metal-dielectric stacks allow these meta-absorbers to have almost perfect absorption throughout the solar spectrum. By the terms metallic patterns and dielectric, we are referring to nano-textures of conventional metals (such as gold, silver, aluminum, and nickel) and well-known dielectric compounds (for example TiO_2 , SiO_2) respectively. This terminology will be used throughout this article. The presence of a metallic pattern or thin metal films within the active layer causes increased recombination of the electron-hole pairs at the metal interfaces [31] in addition to ohmic losses [32] if directly used in a TFSC. Metasurfaces with active layers comprising Group IV materials and III-V compounds can solve these issues. There have been several reports of such broadband meta-absorbers mainly for the infrared regime [33–35]. Vismara et al. proposed a Si nanodisk pattern-based metasurface for solar energy harvesting [36]. However, broadband absorption of the solar spectrum is difficult to achieve in metasurfaces without metallic patterns, quantified by the poor absorption efficiency in their work. All these issues have hindered the direct incorporation of meta-absorbers in solar cells. To the best of our knowledge, a solar cell with a metasurface-based absorber directly incorporated has not been reported yet.

In this article, we propose a novel high-efficiency single-junction thin-film solar cell based on a metasurface absorber. We have used an interconnected dual inverted split ring resonator pattern in a film of InAsP for our absorber metasurface layer, that allows us to overcome the limitations of previously reported metasurface solar absorbers. The absence of metallic patterns or layers in the solar absorber allowed us to directly integrate it into the PV cell, avoiding the unwanted carrier recombination effect. We have separately investigated the absorption characteristics of the metasurface-based absorber in this work, and a peak ideal short circuit current density of $76.23\text{mA}/\text{cm}^2$ was calculated from the optical simulation results. This value is higher than any other Group IV material and III-V compound based absorber structures reported to date [25,26,36–39], allowing our structure to overcome the limitations of such meta-absorbers. This excellent spectral response resulted in an enhancement in power conversion efficiency (PCE) of more than 36% when used as the absorber layer compared to a bare InAsP absorbing layer even without a metallic pattern in the former. This proves the great potential of metasurface absorbers to produce high-efficiency TFSCs. This absorption characteristic, when combined with pyramid-shaped TiO_2 anti-reflecting coating, relatively transparent Indium tin oxide electrode, and a textured back surface in the final structure, produced a 95% absorption band of 400nm to $1.45\mu\text{m}$. The excellent absorption feature translated into a final PCE of 30.87% upon considering different non-idealities in electrical simulations. This is the highest PCE among previously reported III-V single-junction solar cells. Based on the performance of our novel device, it is expected that integrating novel meta-devices in solar cells will go a long way in meeting the global need of high efficiency solar cells for solar energy harvesting.

2. Metasurface based single junction solar cell structure

The configuration of different layers of our proposed metasurface-based single junction thin film solar cell (TFSC) has been schematically shown in Fig. 1(a). We have incorporated the $\text{InAs}_{0.25}\text{P}_{0.75}$ metasurface as the absorber of our solar cell, in contrast to previous literature where the texture has been used only in top and bottom layers as anti-reflecting coating (ARC) or light incoupler and structured back reflector respectively to enhance the photon absorption in the primary absorber layer [12,40–42]. Our metasurface layer has a dual inverted split ring resonator (ISRR) like pattern [43], with both the inner and outer rings interconnected. The cross-section of the absorber layer is depicted in Fig. 1(b). We have used pyramid-shaped TiO_2 ARC over the indium tin oxide (ITO) front electrode and a structured aluminum (Al) back reflector to enhance the absorption in the active layers. The Al nanoparticles (NP) of the back electrode form a 2D grating embedded in the bottom $\text{InAs}_{0.25}\text{P}_{0.75}$ layer.

We have simulated the solar cell structure using Lumerical FDTD Solutions and Lumerical CHARGE solver. The former was used to investigate the optical properties of the structure. For

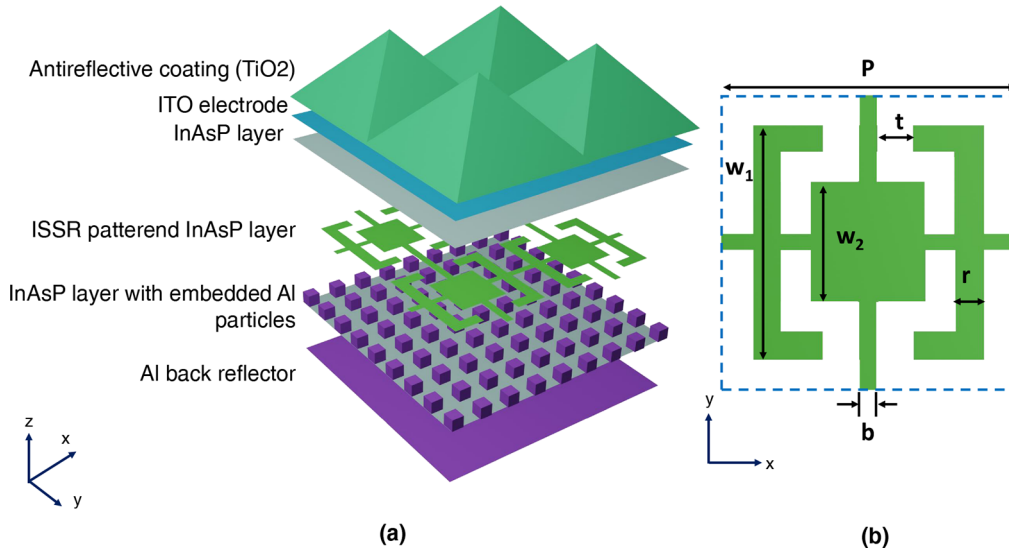


Fig. 1. (a) 3D schematic view of different layers of our proposed metasurface-based solar cell. The figure is not drawn to scale and is a simple artistic depiction of the layer configurations. Starting from the bottom along the z-axis, we have the patterned Al back reflector, which also acts as one of the electrodes, followed by an $\text{InAs}_{0.25}\text{P}_{0.75}$ layer with Al nanoparticles (the 2d grating of the back reflector) embedded at the bottom of the layer. Then we have the ISSR patterned $\text{InAs}_{0.25}\text{P}_{0.75}$. On top of that, we have another plain $\text{InAs}_{0.25}\text{P}_{0.75}$ layer for doping, the indium tin oxide (ITO) electrode, and finally, the pyramid-shaped TiO_2 anti-reflective coating. (b) x-y plane cross-sectional view of the metasurface absorber layer with different structural parameters marked. The blue dashed line indicates the boundaries of a single unit cell, with P being the periodicity. w_1 and w_2 indicate the widths of the inner and outer rings, respectively. The widths of the splits and the rectangles interconnecting the two rings are represented by b and t , respectively. r is the separation between the two rings.

this, a broadband plane wave source propagating along the $-z$ direction was used to illuminate the solar cell, with periodic boundaries along the x and y directions and PML along the z -axis. We calculated the spatial generation rate (G) from the optical simulations for the standard global tilt AM1.5 spectra [44]. The generation values were fed into the CHARGE solver to evaluate the electrical properties of the solar cell. We used the Palik model for the optical properties of the Al electrode [45]. For $\text{InAs}_{0.25}\text{P}_{0.75}$ refractive index data, the values reported by Othman et al. [46] have been used. The refractive index data for ITO and TiO_2 have also been taken from previous literature [47,48]. For the electrical properties of Al and $\text{InAs}_{0.25}\text{P}_{0.75}$, the built-in models of the CHARGE solver were used. We have incorporated the default auger, radiative, and SRH recombination models of $\text{InAs}_{0.25}\text{P}_{0.75}$ in our electrical simulations. A surface recombination velocity of 10^7 cm/s was also considered for this material, keeping in mind the doping concentration used [49]. We have used 4.28 eV as the work function of the ITO electrode in line with previous reports [50].

The choice of mole fraction of the InAsP layers has been driven by the fact that InAs has better absorption characteristics in contrast to the better electrical response of InP. We selected the final mole fraction to maximize the solar cell efficiency. We chose the pyramid shape for the anti-reflecting coating for its polarization and angle-insensitive reflection prevention characteristics [51]. TiO_2 was chosen as it has a high refractive index and low extinction coefficient in the visible to near-IR regime [52], along with excellent chemical and photo-stability

[53]. Pyramid shaped TiO_2 ARC has shown great ability to reduce the unwanted reflection from the top surface in previous reports [51,54,55], enhancing the efficiency of the solar cell. The interconnected dual ISRR has been used for the absorber layer to overcome the inherent low efficiency of Group IV material and III-V compound-based metasurface solar absorbers as it produces better performance compared to single ISRR structure. The field enhancement achieved due to the interaction of the two split rings and capacitive effect induced by the interconnecting rectangles (the air regions of thickness t in Fig. 1(b)) results in an improved absorption performance compared to previous literature. This will be further elaborated in Section 3.2. We have tuned the dimensions of different layers to maximize the ideal short circuit current density ($J_{sc,i}$) of the proposed photovoltaic device found from optical simulations. $J_{sc,i}$ has been used to optimize structural parameters of solar cell in previous literature [56]. The doping concentrations have been chosen to maximize the PCE in the CHARGE simulation. The thickness of the back electrode (h_1) has been kept constant at 300nm during the optimization process to minimize the transmission through the structure for the incident frequencies of concern. Fig. S11, S12, and S13 of the Supplement 1 show the results of tuning different structural and doping profile parameters to obtain the final device. The ideal short circuit current density is calculated from the absorption spectrum using the following formula [37], under the assumption that all the absorbed photons generate electron-hole pairs collectible at the external terminals.

$$J_{sc,i} = q \int_{\lambda_1}^{\lambda_2} \frac{\lambda}{hc} A(\lambda) I_{AM1.5}(\lambda) d\lambda \quad (1)$$

The integration limits have been set to 400nm and $2\mu\text{m}$. q , h , and c represent the electron charge, Planck's constant, and speed of light, respectively. $A(\lambda)$ is the absorption of the structure. $I_{AM1.5}(\lambda)$ is the frequency-dependent incident solar intensity on the US continent obtained from the global tilt AM1.5 data [44]. Different parameters of the structure and doping profile of the optimized device are shown in Table 1 and Table S1 in the Supplement 1, respectively.

Table 1. Different structural parameters for the optimized solar cell structure

Properties	Dimension(nm)	Properties	Dimension (nm)
Al back reflector thickness (h_1)	300	P	361
Bottom InAsP thickness (h_2)	200	w_1	287.5
Al particle height	100	w_2	144
Al particle width	45	r	30
Al particle array period	60.167	b	10
Top InAsP thickness	10	t	41.9
Metasurface layer thickness (h_3)	2650		
ITO electrode thickness	50		
TiO_2 pyramid height	600		
TiO_2 pyramid array period	361		

Several previous works show the feasibility of our proposed solar cell structure. Based on these works we propose a possible methodology for the fabrication of the structure. However, the hands-on fabrication of the device is beyond the scope of this work. The bottom two $\text{InAs}_{0.25}\text{P}_{0.75}$ layers can be grown on an InP substrate using the metalorganic chemical vapor deposition (MOCVD) method [57]. This InAsP layer can then be transfer printed to a textured Al surface. This method has been widely used for III-V compounds [58–60]. After patterning the ISRR onto the InAsP layer, a bare InAsP layer can be transfer printed on top of the patterned layer. Oblique angle deposition has been used in previous works as a suitable technique for depositing the ITO electrode on the InAsP layer [61]. Finally, a TiO_2 layer can be formed using magnetron

sputtering [62], on which pyramid-shaped patterns can be created using soft imprint lithography method [63].

3. Spectral response of the metasurface based solar absorber

We have analyzed the spectral response of the metasurface absorber layer, which is the key to the excellent PCE shown by our proposed photovoltaic structure. To get a better insight into the properties of the metasurface itself, we have omitted the ARC, NPs, and the top InAsP and ITO layers from our final proposed TFSC in Fig. 1(a), which results in a three-layer metasurface-based solar absorber. This structure will be designated as our solar absorber structure throughout the rest of this article. One unit cell of this absorber is shown in Fig. 2(a). The top layer has the same ISRR pattern as in Fig. 1(b). Throughout the analysis in this section, the structural parameters of the optimized final device have been used (Table 1).

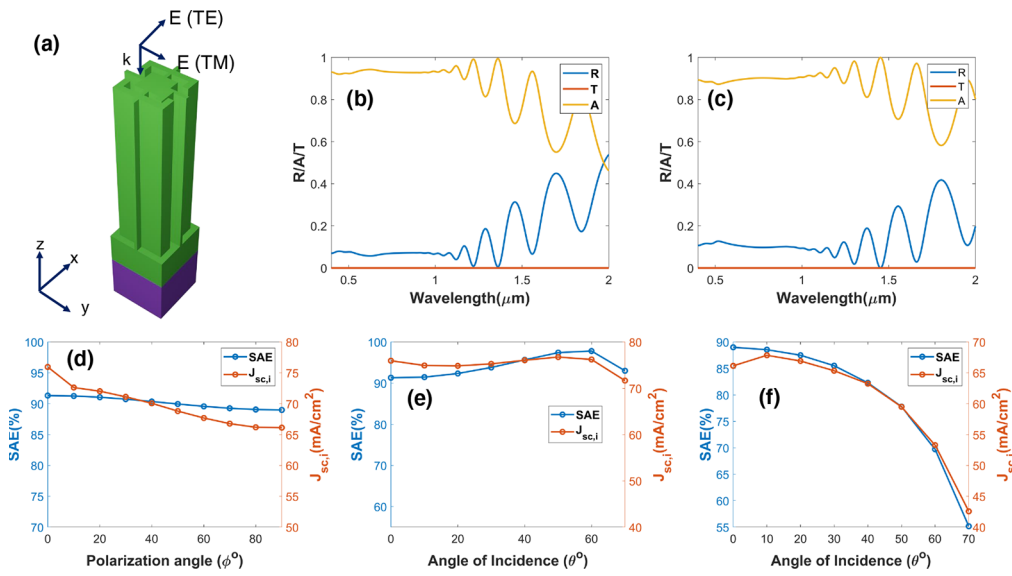


Fig. 2. (a) The 3D schematic view of a unit cell of the inverted split ring resonator-based absorber. The k-vector represents the propagation direction of the EM wave. The two E vector directions correspond to polarization of the electric field for TE and TM polarization. Reflection (R), transmission (T), and absorption (A) spectra for the ISRR based meta-absorber under normal incidence for (b) TE and (c) TM polarization. Variation of the solar absorption efficiency (SAE) and ideal short circuit current density ($J_{sc,i}$) of the absorber for different (d) polarization with normally incident wave and incidence angles for (e) TE and (f) TM polarization.

Our solar absorber structure with a metal back reflector and a top patterned layer (Fig. 2(a)) has a similar configuration as of a typical meta-absorber for solar energy harvesting applications reported in previous literature. However, metasurface based solar absorbers found in prior reports almost invariably contain either patterns or interfaces of well-known metals (like aluminum, silver, gold) with dielectric stacks in the main absorber layer to enhance light-matter interaction [22–30]. The presence of a metallic layer in the active region will result in poor electrical efficiency due to increased carrier recombination at the metal interfaces and ohmic losses [31,32], making such absorbers unsuitable for direct integration into solar cells. In contrast to these conventional absorber systems, our designed metasurface-based structure produces comparable absorption performance without the need for presence of conventional metals either as nano-textures or thin films in the active layer, and also overcoming the low solar absorption

efficiency of Group IV element and III-V compound-based meta-absorbers [36]. This feature of the designed meta-absorber allowed us to design a high-efficiency TFSC directly incorporating the metasurface layer.

3.1. Absorption characteristics

We have numerically studied the optical response of the ISRR based solar absorber using the finite-difference time-domain (FDTD) method in the commercial software Lumerical FDTD Solutions. In the FDTD simulation setup, a plane wave source traveling in the -z direction illuminates the structure as illustrated by the k vector in Fig. 2(a). The transverse electric (TE) and transverse magnetic (TM) polarization refer to EM waves with electric fields in the x and y directions respectively as shown in Fig. 2(a). We used periodic boundaries in the x and y directions and a PML boundary condition along the third dimension. Two 2D frequency domain monitors recorded the transmission (T) and reflection (R). The absorption (A) of the metasurface is calculated using the relation $A = 1 - R - T$ [64,65]. We have also calculated the solar absorption efficiency (SAE) and ideal short circuit current density ($J_{sc,i}$) from the spectral response data. SAE and $J_{sc,i}$ serve as good performance indicators of a solar absorber. $J_{sc,i}$ is defined as in Eq. (1) and SAE is defined as [66]

$$SAE = \frac{\int_{\lambda_1}^{\lambda_2} A(\lambda) I_{AM1.5}(\lambda) d\lambda}{\int_{\lambda_1}^{\lambda_2} I_{AM1.5}(\lambda) d\lambda} \quad (2)$$

Here, the integration limits λ_1 and λ_2 have been set to 400nm and $2\mu\text{m}$ in our calculations. $A(\lambda)$ is the absorption of the solar absorber. $I_{AM1.5}$ is the frequency-dependent incident solar intensity on the US continent obtained from the global tilt AM1.5 data [44].

Figure 2(b)-(e) show the absorption characteristics of the solar absorber, with the same structural parameters as in Table 1. The transmission remains negligible throughout the band for both polarizations due to the thick Al layer used. For TE polarization, under normal incidence, absorption remains above 90% throughout the 400nm to $1.25\mu\text{m}$ band (Fig. 2(b)). This results in an SAE of 91.33% and a short circuit current density of $73.62\text{mA}/\text{cm}^2$. Under normally incident TM polarized wave, these values are 89% and $66.14\text{mA}/\text{cm}^2$ respectively. SAE decreases gradually from 91.33% to 89% as the polarization changes from TE to TM for normally incident EM wave (Fig. 2(d)). For TE polarization, SAE remains above 90% up to an incidence angle of 70° , with a peak value of 97.81% at 60° . This translates into a peak $J_{sc,i}$ of $76.23\text{mA}/\text{cm}^2$ (Fig. 2(e)). This value is higher than those previously reported for Group IV material and III-V compound-based absorber structures [25,26,36–39]. The excellent absorption performance of the metasurface without a layer or pattern of conventional metals reiterates its suitability to be directly incorporated as the absorber layer in a high-efficiency solar cell. However, Under TM polarization SAE is above 80% only upto an incidence angle of 40° (Fig. 2(f)). The absorption performances under varying angles of incidence are quite different for TE and TM polarization as shown in Fig. 2(e) and (f) respectively. One reason for such polarization-sensitive behavior may be the absence of four-fold symmetry in the unit cell, that is we do not get the same initial unit cell upon a 90° rotation. Polarization insensitivity has mainly been observed in structures with four-fold symmetry in previous literature [67–69].

3.2. Electromagnetic field analysis

In order to have a better insight into the absorption characteristics, we have simulated the electric field, magnetic field, and current distributions at different frequencies as shown in Fig. 3 and 4. These quantities are interlinked and can be explained using the well-known Maxwell's equations for EM waves. At the wavelength of 497.5nm, there is a high electrical field at the upper and lower gaps caused by the interconnecting rectangles (air regions with thickness t in Fig. 1(b)), as

shown in Fig. 3(a). This is due to the capacitive effect at the gaps [70]. The high surface current at this wavelength around these regions (Fig. 4(d)) means more charge is stored around the air gap, resulting in a large electric field [71]. This large current also produces a large magnetic field at the edges of the interconnecting rectangles, as can be seen in Fig. 4(a).

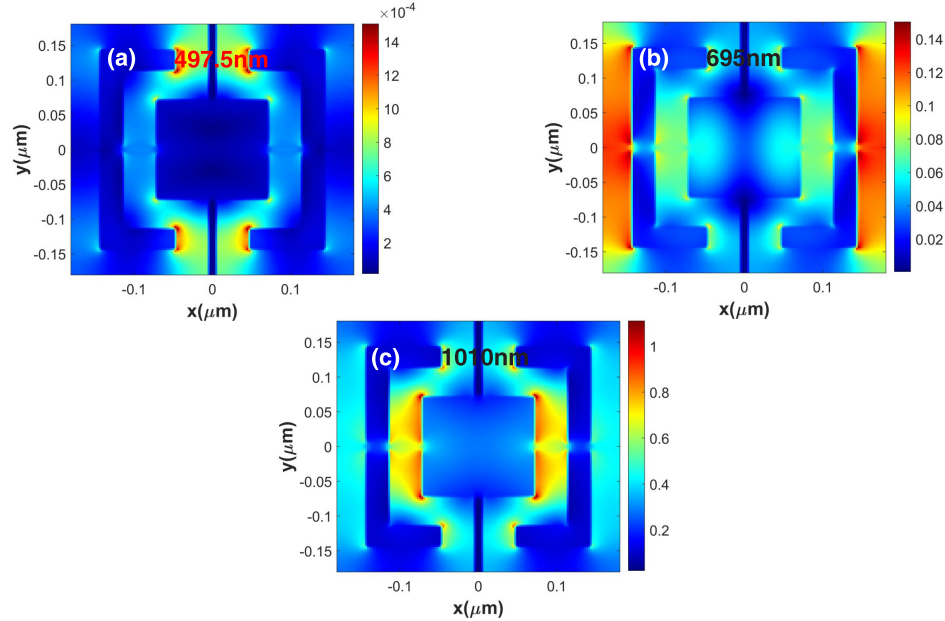


Fig. 3. The x-y plane electrical field distribution of the unit cell at (a) 497.5nm, (b) 695nm, and (c) 1010nm wavelength, under normally incident TE polarized light. The magnitudes of the total electric field have been normalized by the incident field magnitude. All the cross-sectional planes are positioned at a distance of $1.28\mu\text{m}$ along the negative z-axis from the top surface of the patterned InAsP layer.

The current distribution at the 695nm wavelength are depicted in Fig. 4(e). The current around the $y=-0.05\mu\text{m}$ and $y=0.05\mu\text{m}$ planes in the inner InAsP block flow in the opposite direction to the current at around $y=-0.12\mu\text{m}$ and $y=0.12\mu\text{m}$ in the outer block. This results in a small magnetic field in these portions of the meta-atom (Fig. 4(b)). However, high values of parallel surface currents around the $y=0$ plane result in a high magnetic field in the inner block, as illustrated in Fig. 4(b). The strong currents around the splits (the InAsP splits with thickness b in Fig. 1(b)) produce strong electric fields at the inner and outer InAsP blocks around $y=0$ plane (Fig. 3(b)).

At 1010nm, the currents are mainly concentrated at the inner InAsP block in a parallel configuration. This produces a large magnetic field in this block, as can be seen in Fig. 4(c). This strong current concentration at the edge of the inner split produces a high electric field due to the previously mentioned capacitive effect.

To get a better insight into the contribution from different parts of the metasurface pattern, we simulate the absorption spectrum of five different structures, shown in Fig. 5(b), by decomposing the dual interconnected ISRR pattern into its components. The results have been illustrated in Fig. 5(a) and (c). For these simulations, the structural parameters of the optimized system have been kept constant. We have conducted a detailed investigation of the field profiles for cases 2-4 in Fig. S1-S3 of the Supplement 1. The absorbed optical power per unit volume and the solar generation rate distributions for cases 1-5 have also been analyzed in Section 5 of the

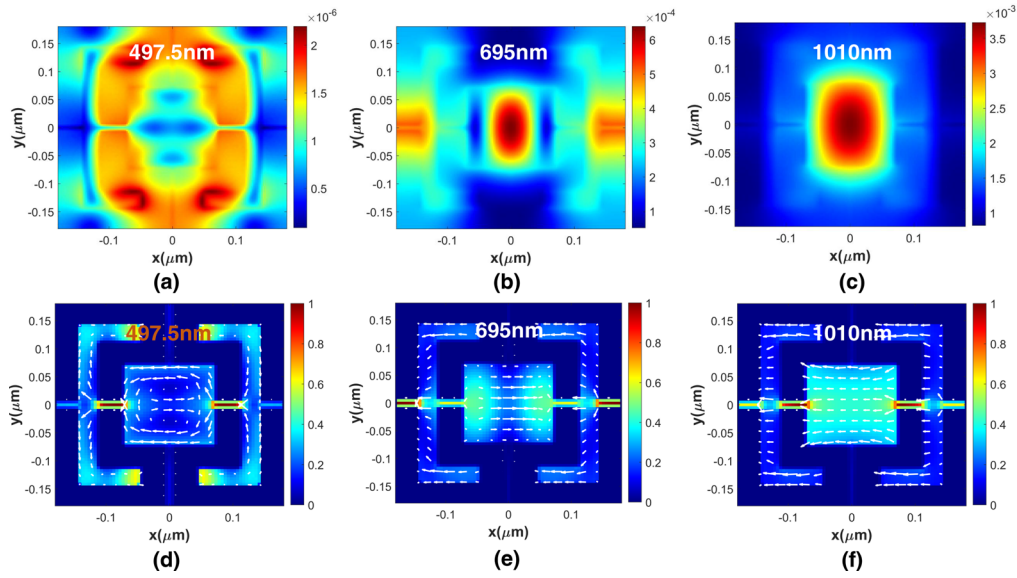


Fig. 4. The x-y plane magnetic field distribution of the unit cell at (a) 497.5nm, (b) 695nm, and (c) 1010nm, under normally incident TE polarized light. The magnitudes of the total magnetic field have been normalized by the incident field magnitude. Current density profile in the x-y plane at (d) 497.5nm, (e) 695nm, and (f) 1010nm. The current density at each wavelength has been normalized with respect to the corresponding maximum values. All the cross-sectional planes are positioned at a distance of $1.28\mu\text{m}$ along the negative z-axis from the top surface of the patterned InAsP layer.

Supplement 1. The absorbed optical power per unit volume is defined as the amount of power absorbed per unit volume (See Section 5 of the Supplement 1 for detailed equation).

The bare InAsP top layer (Case 1) shows reasonable absorption characteristics due to the high extinction coefficient of the material. However, the absorption is quite small, particularly in the smaller wavelength regime, resulting in an SAE and $J_{sc,i}$ of 64.85% and 40.25mA/cm² respectively. Adding an inverted split ring significantly improves the absorption characteristics (Cases 2 and 3). Incorporating both the rings in the same structure (Case 4) improves the absorption further, specifically in the 600-800nm wavelength region as depicted in Fig. 5(a). This is due to the field enhancement caused by the interaction of the two rings, as we explained previously. This improvement is evident in the increase of generation rates and absorbed optical power per unit volume in Case 4 compared to Case 2 and 3 at the 695nm wavelength (See Section 5 of Supplement 1). Interconnecting the two rings with rectangular holes gets us to the final proposed absorber structure (Case 5) with an SAE and $J_{sc,i}$ of 91.33% and 73.62mA/cm² respectively. The high electric field concentration around the interconnecting rectangles in Case 5 at lower wavelengths due to the previously discussed capacitive effect (Fig. 3(a)) results in a significant improvement in the absorption characteristics at these frequencies. This is further verified by investigating the distribution of the absorbed optical power per unit volume in Fig. S9(d) of the Supplement 1. This enhancement in the smaller wavelengths achieved by interconnecting the two rings along with the interaction between the two split-rings at 600-800nm wavelength regime translates into a 40.83% and 82.9% improvement in SAE and $J_{sc,i}$ respectively for Case 5 compared to Case 1.

For completeness, we have also simulated the optimized complementary structure. The structure better resembles a traditional split-ring resonator with InAsP and air interchanged in our absorber structure. This complementary metasurface platform has an SAE of 90.5% and

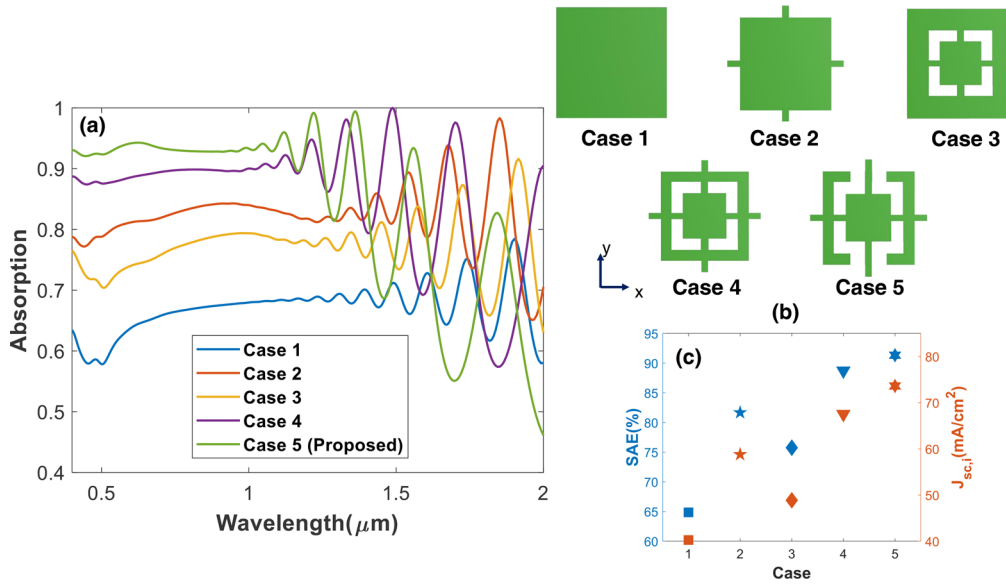


Fig. 5. (a) Absorption spectra for different cases of the top layer in the absorber structure. Case 1 represents bare InAsP as the top layer. Case 2 and 3 have the outer and inner inverted split rings patterned in the top InAsP respectively. For Case 4 both the rings are present. Case 5 corresponds to the actual proposed absorber with interconnected ISRR top layer. (b) x-y plane schematic cross-section of the top layer for the five cases. (c) Values of SAE and $J_{sc,i}$ for the five cases, calculated from the optical simulations.

$J_{sc,i}$ of 57.46 mA/cm² under normally incident TE polarized light. Though the SAE value is slightly lower than our proposed absorber design, the value of $J_{sc,i}$ is 28.1% smaller for this complementary structure, further justifying our use of the ISRR pattern. The optical response of this structure has been depicted in Fig. S4 of the [Supplement 1](#).

4. Optical and electrical properties of the proposed solar cell

To get a better idea of the origin of the excellent efficiency of our proposed single-junction TFSC, we have analyzed four different configurations, as schematically shown in Fig. 6. The first configuration (SC-A) has a bare InAsP absorbing layer. Figure 6(b)-(d) shows the different variations of the metasurface absorber-based solar cell (MSC) and are designated as MSC-B, C, and D, respectively. MSC-D is our final proposed configuration as described in Section 2. For all the variants, the structural and doping parameters have been kept constant as that of the optimal structure (Table 1 and Table S1 in the [Supplement 1](#)). We have simulated the optical and electrical characteristics of all four configurations. From the FDTD simulations, the absorption spectra, SAE, and $J_{sc,i}$ have been obtained. These parameters are an estimate of the amount of electron-hole pairs generated in the structure. However, all these electron-hole pairs are not collected in the electrodes and do not contribute to the final output power. For this, we have also simulated the electrical characteristics of all three MSCs along with the bare absorption layer variant (SC-A) considering different non-ideal effects as described in Section 2. From the electrical simulations, we have obtained the short circuit current density (J_{sc}), fill factor (FF), open circuit voltage (V_{oc}), and PCE. FF has been defined using the following equation [72]

$$FF = \frac{P_{max}}{J_{sc} V_{oc}} \quad (3)$$

where, P_{max} is the maximum output power per unit area.

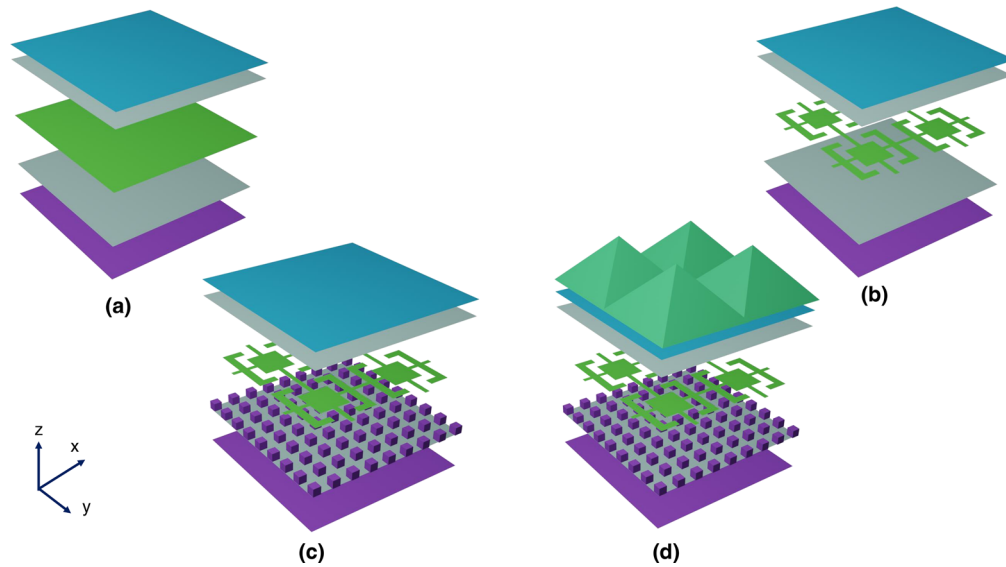


Fig. 6. The composition of different layers of the four solar cells simulated. (a) SC-A consisting of an Al back reflector, three $\text{InAs}_{0.25}\text{P}_{0.75}$ layers with different doping configurations, followed by ITO electrode at the top. The middle InAsP layer is the absorbing layer. (b) MSC-B structure with the ISRR-based absorber as the absorbing layer. (c) MSC-C composition, with a 2D array of Al nanoparticles embedded in the bottom InAsP layer, in addition to the ISRR-based metasurface on top of this layer. (d) schematic of the MSC-D structure, our final proposed solar cell. This structure has a similar configuration as the MSC-C. However, there is an additional pyramid-shaped TiO_2 array on top of ITO, acting as an ARC.

Figure 7, 8, and 9 respectively illustrate the optical, J-V, and P-V characteristics of the four structures. The spatial distributions of the electrical generation rate for standard AM1.5 solar power spectra of all the structures have been shown in Fig. S5 of the Supplement 1. For SC-A configuration with bare InAsP as the absorber layer, the absorption is relatively low at higher wavelengths, as shown in Fig. 7(a). This is mainly due to the bandgap limitation of the material and significant reflection from the ITO electrode. From the absorption plots, the values of SAE and $J_{sc,i}$ have been calculated to be 80.3% and $46.93\text{mA}/\text{cm}^2$, respectively. This poor absorption characteristic results in a relatively small PCE of 19.25%, as can be calculated from Fig. 9(a).

In the case of MSC-B, where we have included our designed metasurface-based solar absorber, has better optical characteristics than SC-A, quantified by a higher SAE (86.97%) and $J_{sc,i}$ ($64.88\text{mA}/\text{cm}^2$). However, the optical performance is inferior to the metasurface absorber described in Section 3. This is again due to the presence of ITO and InAsP on top of the proposed solar absorber. Though we have used thin layers for the top InAsP and ITO, they respectively cause partial absorption and reflection of the incident wave before entering the metasurface. MSC-B has a PCE of 26.32%, which is about 36.8% higher than the structure with bare InAsP (SC-A). This variant has a fill factor, open circuit voltage, and short circuit current density of 0.87, 0.68V, and $44.35\text{mA}/\text{cm}^2$ as can be seen from the J-V and P-V characteristics in Fig. 8(b) and 9(b) respectively. All these values are higher than SC-A, quantifying the significance of the pattern structure in our final device.

In the third solar cell variant under consideration (MSC-C), we have incorporated an array of Al nanoparticles in the bottom InAsP, which can also be interpreted as using a structured back

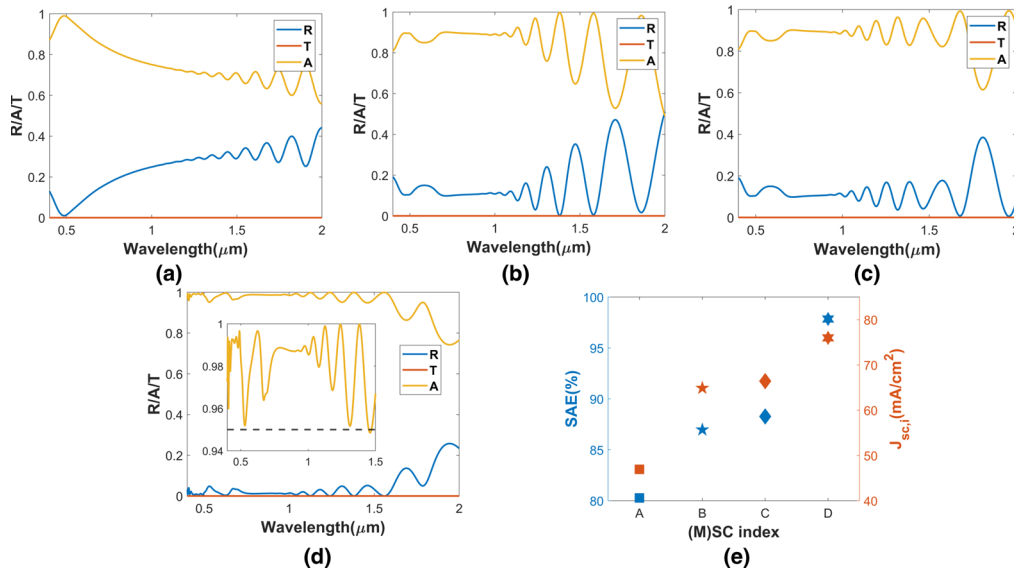


Fig. 7. Reflection (R), transmission (T), and absorption (A) spectra of (a) SC-A, (b) MSC-B, (c) MSC-C, and (d) MSC-D. The inset in (d) gives an enlarged view of the variation of A for MSC-D. The dotted line represents 95% absorption. (e) Variation of SAE and $J_{sc,i}$ for the four configurations.

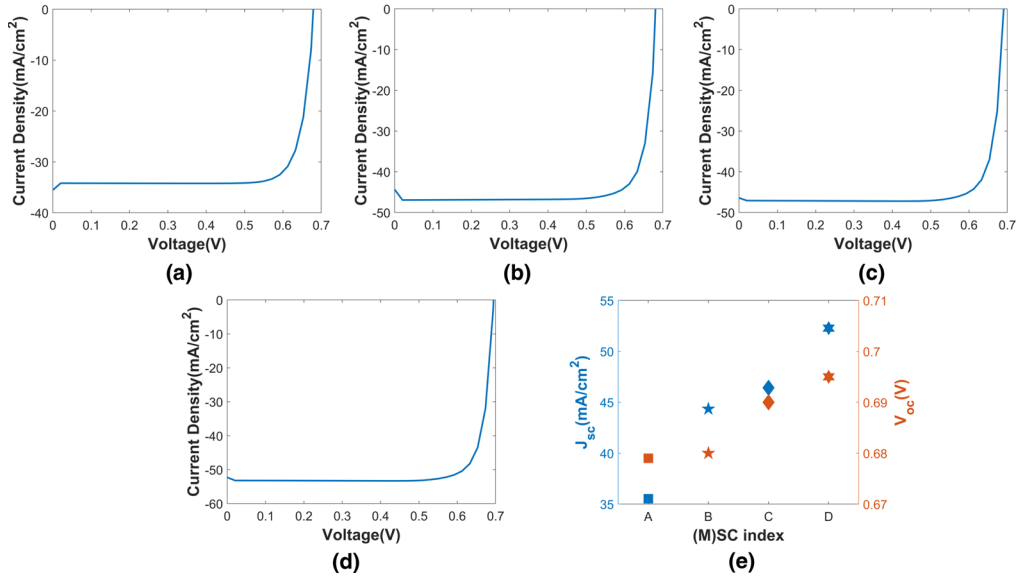


Fig. 8. Current density (J) vs voltage (V) characteristics of (a) SC-A, (b) MSC-B, (c) MSC-C, and (d) MSC-D. (e) Variation of J_{sc} and V_{oc} for the four configurations.

reflector(Fig. 6(c)). We have used the 2D configuration for the array, which has been found to produce better absorption enhancement in previous literature [42]. This array of particles acts as a two-dimensional grating and scatters laterally traveling waves in the bottom InAsP layer, resulting in an increased absorption. Incorporating the nanoparticle array results in an increased

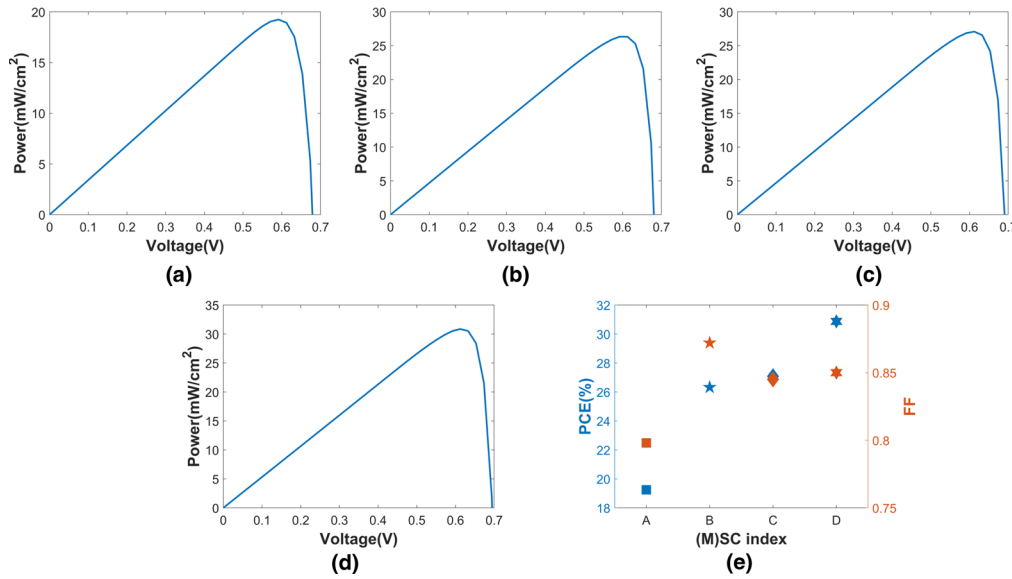


Fig. 9. Power vs voltage (V) characteristics of (a) SC-A, (b) MSC-B, (c) MSC-C, and (d) MSC-D. (e) Variation of PCE and FF for the four configurations.

absorption in the IR regime (Fig. 7(c)) compared to SC-A and MSC-B. This results in a slightly improved PCE of 27.08%.

Our final proposed solar cell configuration, MSC-D, has much improved optical absorption characteristics than the three previous variants, as depicted in Fig. 7(d). The inset of the figure shows an absorption of larger than 95% throughout the 400nm to 1.45 μ m spectral band. This structure has an SAE of 97.86% and $J_{sc,i}$ of 76.01mA/cm², which is significantly higher than the previous configurations. This improvement is mainly due to the use of a pyramid-shaped TiO₂ array as the anti-reflection coating. This reduces the reflection of incident light from the ITO electrode. This excellent optical performance translates into a record PCE of 30.87% for III-V material-based solar cells calculated from the P-V characteristics in Fig. 9(d). This MSC has a fill factor, open circuit voltage, and short circuit current density of 0.85, 0.695V, and 52.28mA/cm², respectively.

Table 2 summarizes the optical (SAE, $J_{sc,i}$) and electrical (V_{oc} , J_{sc} , FF, PCE) performance parameters of the four configurations. The performance gradually improves from SC-A to MSC-D, quantified by the relative PCE. The final proposed structure (MSC-D) has an improvement of 60.4% in PCE compared to the structure with bare InAsP (SC-A). Also, it is worth noting that the ideal short circuit currents ($J_{sc,i}$) calculated from the FDTD simulations decrease in the currents (J_{sc}) calculated from the CHARGE solver for all the devices due to the non-ideal effects incorporated. The decrease is prominent in the metasurface-based solar cells (MSC-B, MSC-C, MSC-D) compared to the unpatterned structure (SC-A). The patterns in the former configurations may have deteriorated the electrical performance compared to the latter and requires further investigation. We have compared the electrical performance of our proposed metasurface absorber-based solar cell (MSC-D) structure with previously reported single-junction III-V solar cells in Table 3. The table includes high efficiency single junction III-V solar cells, irrespective of numerical and experimental investigation conducted. For clarity, we have indicated which of the efficiencies are experimentally verified. Our device shows a relative enhancement in PCE of 6.1% compared to the maximum reported value of 29.1% for III-V SCs. The excellent

performance of this novel TFSC configuration will pave the way for incorporating metasurfaces in future high-efficiency solar cell applications.

Table 2. Comparison of the optical and electrical performance of the four configurations

Structure	SAE(%)	$J_{sc,i}$ (mA/cm ²)	V_{oc} (V)	J_{sc} (mA/cm ²)	FF	PCE(%)	Relative PCE
SC-A	80.271	46.934	0.679	35.526	0.798	19.243	1
MSC-B	86.968	64.883	0.680	44.347	0.872	26.323	1.368
MSC-C	88.271	66.432	0.690	46.423	0.845	27.078	1.407
MSC-D	97.855	76.013	0.695	52.280	0.850	30.869	1.604

Table 3. Comparison of the electrical performance with previously reported III-V single-junction solar cells

Structure	V_{oc} (V)	J_{sc} (mA/cm ²)	FF	PCE(%)	Reference
InP NW + ITO NP	0.765	29.3	0.794	17.8(experimental)	[5]
ITO-InP + back photonic crystal	0.81	33.1	0.86	25.7(numerical)	[6]
GaAs + AR	1.11	29.6	0.84	27.6(experimental)	[7]
GaAs + Al NPs + Ta ₂ O ₅ ARC	1.103	28.17	0.89	27.66(numerical)	[8]
GaAs TFSC	1.13	29.78	0.87	29.1(experimental)	[73]
MSC-D	0.695	52.280	0.850	30.869(numerical)	This work

5. Conclusion

In this work, we report a metasurface absorber-based single junction thin film solar cell. The use of well-known metals as nano-textures or thin films in conventional solar meta-absorbers has been an obstacle to their direct incorporation as the active absorbing layer in solar cells. We have alleviated this problem by using an inverted split ring resonator pattern in the InAsP active layer of our solar cell. Optical simulations of the metasurface revealed an excellent solar energy absorption capability quantified by the maximum ideal short circuit current density for Group IV material and III-V compound-based solar absorber platforms. This result shows the ability of our metasurface layer to overcome the low absorption efficiency drawback of such meta-absorbers. We have used ARC, a textured back reflector, and a transparent ITO electrode in the final device. These conventional efficiency enhancement methods combined with the metasurface-based absorber layer allowed us to achieve a solar absorption efficiency of close to 98% in the FDTD simulations. This resulted in an overall power conversion efficiency of 30.87% considering different non-ideal effects in electrical simulations, which is 6.1% higher than previously reported maximum PCE for III-V single-junction solar cells. The unprecedented performance of our metasurface-based solar cell will open new avenues for the application of metasurfaces in next-generation high efficiency solar photovoltaic devices.

Disclosures. The authors declare no conflict of interest.

Data availability. Data underlying the findings of this work are not public at this time but will be made available upon reasonable request to the authors.

Supplemental document. See [Supplement 1](#) for supporting content.

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