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Surface Modification of Semiconductor Nanoparticles for Enhanced Optical Performance

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Abstract

Semiconductor nanoparticles, sometimes called quantum dots, have recently gained attention as a possible useful material due to the fact that their optical and electrical properties are size dependant. However, surface-related defects, nonradiative recombination, and limited stability under ambient conditions often limit their practical use in optoelectronic devices, sensors, and bioimaging. By enabling the changing of the physical and chemical characteristics of nanoparticle surfaces, surface modification methods provide an effective way to circumvent these problems. Photoluminescence efficiency, charge carrier dynamics, and environmental stability may all be enhanced by using certain techniques, such as ligand exchange, core-shell engineering, and surface passivation. Organic and inorganic moiety functionalization improves optical performance, opens the door to biocompatibility, and enables selective targeting in biomedical applications, among other benefits. These qualities are crucial for uses in biology, therefore this is significant. The potential of these altered nanostructures in quantum technologies, photocatalysis, light-emitting diodes, and next-generation solar cells has been shown by advances in controlled synthesis and surface engineering. This study aims to investigate how surface modification may be used to enhance the optical properties of semiconductor nanoparticles. The current strategies, fundamental mechanisms, and potential future developments leading to adaptable, stable, and application-ready nanomaterials are the main points of discussion.

Keywords: Semiconductor, Nanoparticles, Surface

Introduction

There is a distinct category of nanomaterials known as semiconductor nanoparticles, which are often referred to as quantum dots (QDs). These nanomaterials are characterised by their optical and electrical characteristics being heavily regulated by quantum confinement phenomena. When the size of a semiconductor crystal is reduced to a few nanometres, which is comparable to or smaller than its exciton Bohr radius, the electronic band structure undergoes a significant transformation. This results in size-tunable absorption and emission spectra, high photoluminescence quantum yields, and remarkable nonlinear optical behaviour. As a result of these qualities, semiconductor nanoparticles are excellent candidates for a wide variety of applications, such as light-emitting diodes (LEDs), lasers, solar cells, photocatalysis, sensors,

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and biomedical imaging. In spite of the enormous potential that they provide, the optical performance of semiconductor nanoparticles is sometimes hampered by the existence of defects associated to the surface environment. The nanoscale is characterised by a significant proportion of atoms that are located on the surface. This results in the formation of dangling bonds and trap states, which function as centres for nonradiative recombination. In the long run, this leads to a decline in photoluminescence efficiency, spectrum widening, and poor long-term stability under ambient circumstances such as exposure to light, heat, and moisture. In light of this, surface modification has emerged as an essential method for releasing the full potential of semiconductor nanoparticles. The term "surface modification" refers to the process of modifying the surface of a nanoparticle using chemical or physical means with the intention of altering the electronic structure, chemical reactivity, and interfacial interactions of the nanoparticle. Extensive research has been conducted on several methods, including ligand engineering, inorganic shell development, polymer encapsulation, and heterostructure synthesis, with the goals of reducing surface trap states, passivating defects, and enhancing colloidal stability. One example is the development of a core–shell nanostructure, which involves the growth of a wide-bandgap shell around a semiconductor core. This helps to confine charge carriers more efficiently, which ultimately leads to improved emission efficiency and stability. In a similar vein, the exchange of ligands with molecules that are either organic or inorganic can result in improved solubility, biocompatibility, and regulatory control of energy transfer.

Recent developments in this area have shown that surface-modified semiconductor nanoparticles are capable of achieving considerable improvements in optical performance. They have been positioned as materials of the next generation for applications linked to energy and optoelectronics as a result of their enhanced quantum yield, decreased blinking, increased charge separation, and prolonged photostability. Additionally, functional surface engineering makes it possible to include nanoparticles into hybrid systems, which enables synergistic effects for advanced device designs. In this research, the fundamental concepts and tactics of surface modification of semiconductor nanoparticles are investigated, with a particular emphasis on the ways in which these changes influence the optical characteristics of the nanoparticle structures. It analyses current achievements, highlights state-of-the-art methodologies, and explores future possibilities in the development of high-performance nanomaterials that are optimised for practical applications in the fields of photonics, energy, and biology.

Surface Defects and Their Impact

It is common for surface defects to have an impact on the characteristic optical capabilities of semiconductor nanoparticles. These capabilities include size-tunable emission and high absorption coefficients. These characteristics include the capacity to absorb light with wavelengths that are quite long. In 1986, Brus was the first person to communicate the concept of quantum confinement to the scientific community. He provided evidence that the size of particles has an impact on the electrical structure of a system when he proved this. He did, however, draw attention to the fact that surface traps at the nanoscale are far more difficult to create. Research that was conducted after that (Alivisatos, 1996; Klimov, 2000) brought to light the fact that unsaturated bonds on the surfaces of nanoparticles serve as nonradiative recombination centres, which in turn reduces the emission efficiency and stability of the particles.

Ligand Engineering

Despite the fact that organic ligands play a vital role in the process of stabilizing nanoparticles in colloidal suspension, the electrical insulating characteristic of organic ligands can slow down charge transfer in device applications. This is because organic ligands have the ability to protect charges from being transferred. Murray and colleagues (1993) were the pioneers in the field of ligand exchange methods, which were developed with the purpose of improving the electrical connection between nanoparticles. The natural long-chain ligands are taken out of the equation and replaced with alternatives that are either shorter or more conductive. These strategies are used. According to research that was carried out not too long ago (Talapin et al., 2010), the incorporation of inorganic ligands, such as metal chalcogenide complexes, has been discovered to lead to a significant improvement in conductivity while simultaneously maintaining optical performance. According to Smith and Nie (2010), functional ligands have also been used for the purpose of accomplishing biomedical targeting and enhancing biocompatibility.

Core–Shell Structures and Passivation

The creation of core–shell structures has shown to be one of the most effective methods for reducing the number of surface trap states. As a result of excellent surface passivation, Dabbousi et al. (1997) revealed that covering CdSe cores with a ZnS shell made a significant improvement in both the quantum yield and the stability of the material. There have been several cores–shell pairings that have been researched since that time (Chen et al., 2013; Protesescu et al., 2015). Some examples of these combinations are CdSe/ZnSe, InP/ZnS, and perovskite-based nanostructures. Not only do these heterostructures improve photoluminescence, but they also inhibit photooxidation and avoid fluorescence blinking.

Polymer and Inorganic Encapsulation

In addition to the modification of ligands and shells, encapsulation through the use of polymers and inorganic matrices provides additional techniques for surface stabilization. Wuister et al. (2003) made the observation that polymer coatings have the potential to improve the water stability and biocompatibility of quantum dots for imaging applications. Similarly, silica encapsulation (Bruchez et al., 1998) has been extensively used for the aim of insulating nanoparticles from oxidative degradation while simultaneously permitting surface functionalization with biomolecules. This has been done in order to achieve the same goal.

Emerging Trends in Surface Engineering

The usual use of passivation has been surpassed by those recent innovations. In spite of the fact that perovskite quantum dots have the potential to be utilized in applications that include light-emitting and light-harvesting, they are exceedingly unstable when they are subjected to heat and moisture. It has been established that surface treatments using ionic ligands (Zhang et al., 2019) and encapsulation approaches (Li et al., 2020) have both exhibited significant increases in terms of stability and luminescence retention. Additionally, hybrid organic–inorganic surface treatments are now being researched in order to combine the advantages of flexibility, conductivity, and stability (Akkerman et al., 2018). This is being done in order to get the desired results.

Applications Driven by Surface Modification

Surface alteration may be observed in a wide range of practical contexts. In photovoltaics, surface passivation improves charge extraction and reduces recombination losses (Nozik, 2002). Ligand and shell engineering is associated with improved light-emitting device brightness and color purity (Shirasaki et al., 2013). Medintz et al. (2005) states that surface functionalization is a method utilized in biomedicine to facilitate cellular imaging and selective targeting. As shown in these specific cases, device-level performance is directly dictated by surface chemistry.

Methods

Producing AgNP films and silver hydroxide nanocomposite at room temperature was achieved through the use of modified electrical etching (EE). The initial step involved spin-coating pure n-type silicon wafers in water with silver nanoparticles. Hydrogen fluoride at 5 M and water with 0.2 M hydrogen created silicon nanoholes (SiNHS) when submerged in the samples. Because of this etching, nanoholes were filled with AgNP deposits. The samples underwent a deionized water cleaning, a nitrogen blast to remove excess moisture, and 1.5 hours of air drying after etching. This method enhanced the bonding of SiOx and Si surfaces. Currently, a nanocomposite layer has created from the combination of silver nanoparticles and silicon nanoholes. Etching duration, AgNP size, and particle distance all had an impact on the film's hole size and spacing. Using SiNHS, AuNPs, and PEDOT:PSS, hybrid solar cells were created after synthesizing the AgNP/SiNHS nanocomposite. The films were spin-coated at 3,000 RPM for 60 seconds after combining PEDOT:PSS with AuNPs in water to generate the heterojunction layer. Magnetron sputtering was used to deposit silver and aluminum electrodes, which were then used to create ohmic substrate connections. Using AFM and SEM, we looked at the materials' morphology. A Shimadzu UV-3600 spectrophotometer was used to evaluate optical absorption at room temperature. The performance of the PV cells was evaluated under 100 mW/cm2 of AM 1.5G light. Aspects of illuminated I-V and EqE spectra from the outside were assessed. The spectral responses of devices were measured experimentally. For the hybrid solar cell structure shown in Figure 1, the components are silver nanoparticles, SiNHS, and AuNP/PEDOT:PSS.

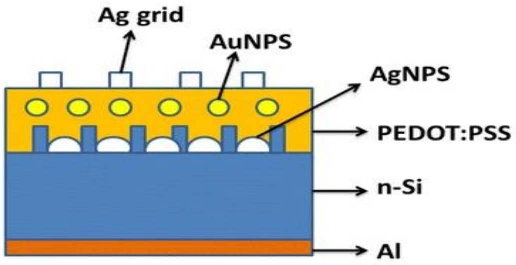

Figure.1: Localized Surface Plasmon Resonance Improves Organic Hybrid Solar Cells with Gold Nanoparticles and Silicon Nanoholes.

Results and Discussion

Nan composite Films of SiNHS/PEDOT: PSS: A Study of Their Structure

The AFM pictures of spin-coated gold nanoparticles (AuNPs) on the flat surfaces of silicon wafers are shown in Figure 2a. The average diameter of AuNPs is 50 ± 5 nm, and they are spherical in shape. In a scanning electron micrograph (SEM) of AgNP/SiNHS nanocomposite films taken from above, silicon nanoholes with a diameter of 150 nm are seen in Figure 2b. Figure 2c shows scanning electron microscopy (SEM) images of cross-sectional SiNHS/AgNP films, which suggest that AgNPs might be accommodated by the SiNHS structure. The cross-sectional scanning electron micrograph (SEM) image of the SiNHS/AgNPs and PEDOT:PSS/AuNPs heterojunction is shown in Figure 2d. According to the images, the samples have a uniform and smooth surface because the PEDOT:PSS/AuNP layer is completely absorbed into the SiNHS matrix.

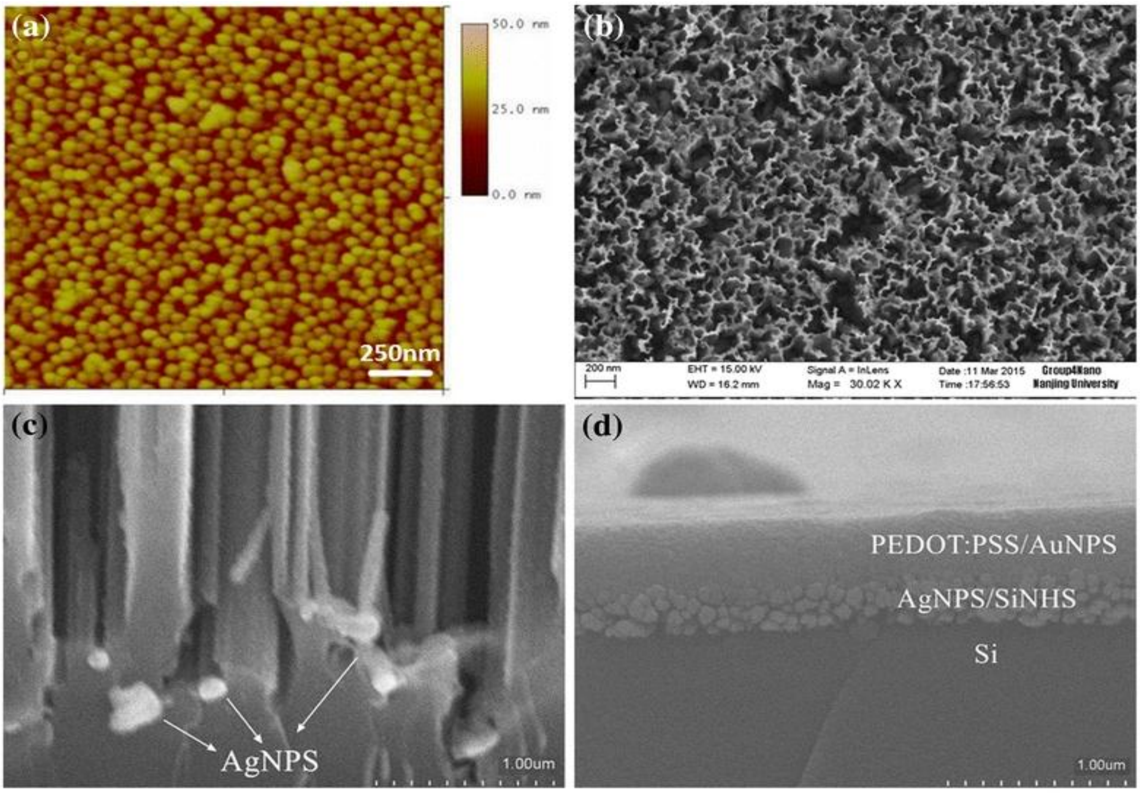

Figure.2: Organic-Silicon Hybrid Solar Cells Achieve Greater Efficiency Through Surface Plasmon Resonance Localization

These gold nanoparticles were captured in an atomic force microscope image. Nanocomposite films of AgNPS and SiNHS are revealed by top-down scanning electron microscopy. Electron microscopy reveals films of nanocomposite materials made of AgNPS and SiNHS. Electron micrographs taken in cross-sectional patterns show sheets coated with PEDOT:PSS/AuNPS.

Solar Cell Efficiency

To investigate the impact of surface passivation on SiNHS-based hybrid heterojunction solar cells, we established a SiOx-Si connection at the organic-silicon interface. Comparing devices without this interfacial change yielded a maximum power conversion efficiency (PCE) of 5.5 percent. Investigated were the J-V properties and EQE of solar cells both with and without surface modification. Figure 3 displays the outcomes. Table 1 shows the outcomes of the tests conducted under AM 1.5G illumination at 100 mW/cm^2 on fill factor (FF), power consumption efficiency (η), open-circuit voltage (Voc_{oc}oc), and short-circuit current density (Jsc_{sc}sc). Devices utilizing SiOx-SiNHS/AgNPS films showed better Jsc_{sc}sc and EQE when compared to devices without passivation. The SiOx-Si passivation layer mitigates surface imperfections and carrier recombination, which impact device performance. In order to decrease light-induced charge recombination between SiNHS and metal nanoparticles, surface passivation is used to form an extremely thin oxide layer. As a result, both the fill factor and PCE increased by 25%. Over a large portion of the visible spectrum, passivated samples exhibit enhanced EQE. Air-grown SiNHS/AgNPS nanocomposite films increased the number of SiOx-Si bonds, which further decreased interface defects. The efficiency of hybrid solar cells was increased by surface passivation, while PCE in organic-silicon heterojunction devices was improved through interfacial engineering of nanocomposite films.

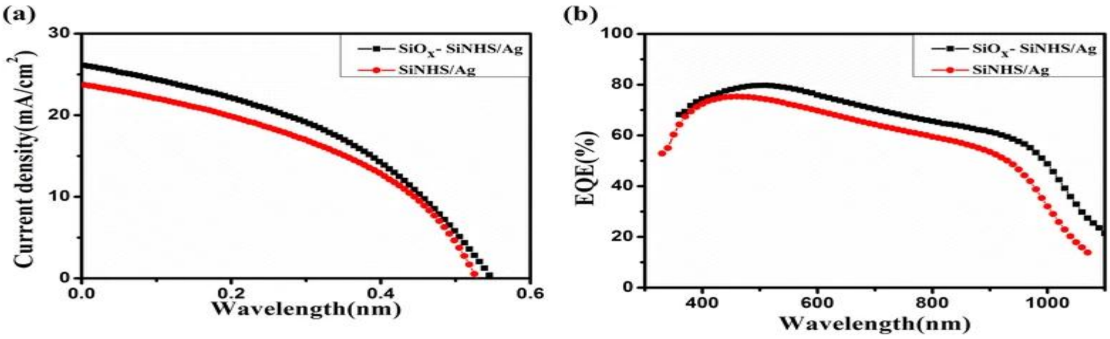

Figure.3: Localized Surface Plasmon Resonance Enhances the Efficiency of Organic Hybrid Solar Cells Containing Gold Nanoparticles and Silicon Nanoholes.

You will receive these settings in a separate package. There was an evaluation of hybrid solar cells with and without a SiOx-Si connection.

Table 1 Comparison of SiOx-Si bond-using and non-using hybrid solar cell systems

Devices	**V oc (V)**	**J sc (mA/cm2)**	**FF (%)**	**PCE (%)**
SiNHS/Ag	0.527	23.6	39.4	4.8
SiOx–SiNHS/Ag	0.538	26.1	41.6	5.5

By using localized surface plasmon resonance, the efficiency of organic hybrid solar cells including gold nanoparticles and silicon nanoholes is further enhanced.

Another aspect that restricts the power conversion efficiency (PCE) of hybrid solar cells is organic silicon's extremely poor efficiency in absorbing light. Recently, there has been a surge in interest in solar cells that utilize the LSPR effect, a phenomenon caused by metal nanoparticles, as a possible remedy for this issue. Researchers found that hybrid heterojunction solar cells' light-trapping efficiency was improved when metal nanoparticles were added to

PEDOT:PSS buffer layers. This was due to an increase in light scattering. Metal nanoparticles, which exist in PEDOT:PSS in a range of LSPR wavelengths, significantly enhance the light absorption.

Gold nanoparticles (AuNPs) were used to improve the total power conversion and light absorption in organic layers made of passivated nanocomposite films. To examine the effect of LSPR on the performance of organic-silicon hybrid solar cells, we set out to examine the light absorption spectra of AuNPs, colloidal AgNPs, and AuNP/SiNHS nanocomposite films. The main objective of the experiment was to determine the effects of LSPR on the optical characteristics and efficiency of the device. We started by taking R and T spectra of the materials using a Shimadzu UV-3600 spectrophotometer. After that, the absorbance (A) spectra were determined by applying the subsequent formula:

$$A=1-T-R.$$

We use fifty spherical gold particles with a diameter of nanometers to maximize the use of gold nanoparticles and enhance the light-absorbing capabilities of solar cells.

Both the AgNPs and the AuNPs' absorption spectra in deionized water are displayed in Figure 4a. In contrast to the 520 nm peak seen for the AuNPs, the AgNPs exhibited an absorption peak at about 480 nm. The localized surface plasmon resonance (LSPR) of the nanoparticles allowed us to detect this peak. Nanocomposite films of AgNP/SiNHS with different compositional properties and mass ratios of AuNP, PEDOT, and PSS are shown in Figure 4b, along with their absorption spectra. The absorption peak was redshifted to around 550 nm as a result of interactions involving charge transfer among the nanoparticles, the silicon substrate, and nearby particles. Another probable cause of this redshift is energy loss as a result of electron-hole interactions with atoms in the lattice. A higher AuNP mass ratio resulted in devices that absorbed more light at wavelengths longer than 600 nm. Better absorption is mainly caused by increased light dispersion inside the films, which is the fundamental reason for this improvement. With a total absorption increase of 16.1% between 300 and 1000 nm, the sample containing 0.5 wt% AuNPs demonstrated the greatest improvement in long-wavelength light absorption when examined using an integrating technique.

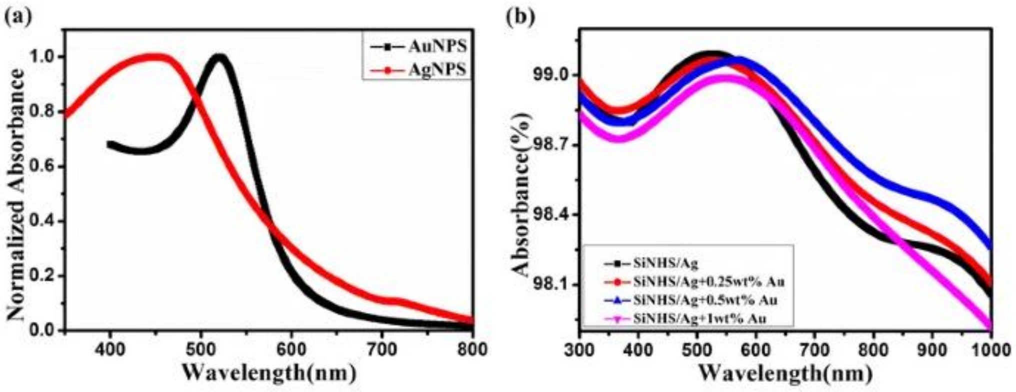

Figure. 4: Localized Surface Plasmon Resonance Enhances the Efficiency of Organic Hybrid Solar Cells Containing Gold Nanoparticles and Silicon Nanoholes.

Displayed here are the optical absorption spectra of AuNPs in a deionized water solution. b Optical absorption spectra of PEDOT films etched for varying times in contrast to films without AgNPs: nanocomposite films containing PSS, AuNPS, AgNPS, and SiNHS By boosting the light absorption capacity of solar cells, the LSPR effect—which may be generated by AuNPS and AgNPS—might prolong the absorption peak of nanocomposite films. The usage of AuNPS may also improve the light scattering characteristics of the devices. At 0.5 weight percent, the maximum quantity of light absorption was achieved by increasing the mass ratio of AuNPS. When the concentration of AuNPS in the devices increased, however, their light-absorbing properties decreased. Having an excessive number of particles on the surface of nanocomposite films would reduce their ability to absorb SiNHS. Our research indicates that a mass ratio of half a weight percent for AuNPS is ideal.

Under simulated AM 1.5 G illumination at 100 mW/cm2 and EQE, we measured the current density-voltage characteristics of films made of PEDOT: PSS/AuNPS/(AgNPS/SiNHS) nanocompoite to determine the impact of metal nanoparticles on hybrid solar cell performance. Table 2 displays many photovoltaic metrics, including V oc, J sc, FF, and PCE.

Table 2 How well hybrid solar cells work, device-wise, with or without AgNPs or AuNPs

Devices	V_{oc} **(V)**	J_{sc} **(mA/cm^2)**	**FF (%)**	**PCE (%)**
SiOx–SiNHS/Ag + Au	0.531	27.3	42.1	6.1
SiOx–SiNHS/Ag	0.541	25.5	40.8	5.5
SiOx–SiNHS	0.501	20.8	22.9	2.4

By using localized surface plasmon resonance, the efficiency of organic hybrid solar cells including gold nanoparticles and silicon nanoholes is further enhanced.

If you look at Figure 5 and Table 2, you'll see that systems with nanoparticles outperformed those without. The gadgets' enhanced capacity to capture light might explain this improvement. Our remarkable light harvesting efficiency was, in theory, caused by the plasmon resonance effect that the metal nanoparticles generated.

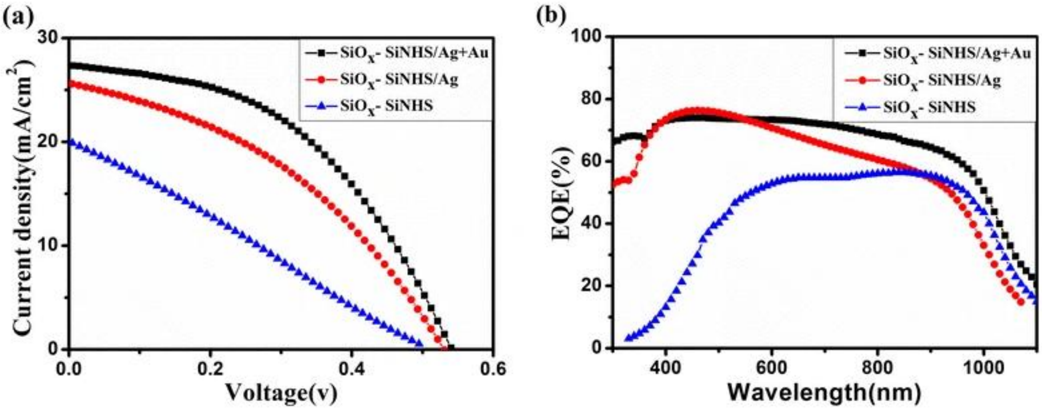

Figure.5: To further improve the efficiency of organic hybrid solar cells, which already contain gold nanoparticles and silicon nanoholes, localized surface plasmon resonance is used.

Figure 5a shows the J-V characteristics of hybrid solar cells with and without AgNPs or AuNPs, whereas Figure 5b shows the comparable EQE spectra. The short-circuit current densities of devices that contained AuNPs were greater than those that did not. Table 2 shows that there was a rise of around 7% in the short-circuit current and an improvement of 5.5% to 6.1% in the power conversion efficiency (PCE). Figure 4a shows that the better light absorption, caused by the fact that AgNPs and AuNPs have different LSPR peak locations, is the reason for the increase in photovoltaic performance. This pattern is further supported by Figure 4b, which indicates that the observed EQE values are remarkably comparable to the absorption spectra of the solar cells. For the simple reason that for wavelengths greater than 600 nm, the EQE values of devices doped with AuNPs are much higher. Photoselective charge separation is made more efficient with the addition of AuNPs because they increase light scattering inside the device and strengthen the local electromagnetic field via the LSPR effect. Our results show that device performance is much enhanced when silicon nanostructures are surface passivated and plasmonic nanoparticles are used together. Metal nanoparticles augmented with light-sensitizing quantum dots (LSPR) increase optical absorption and localized electromagnetic fields, while surface passivation decreases carrier recombination. Light scattering is enhanced by an increase in optical path length, which in turn enhances absorption efficiency. Incorporating SiNHS and AuNPs into organic hybrid solar cells improves their performance.

Conclusions

Utilizing the EE method, hybrid solar cells were finally manufactured utilizing a nanocomposite film including PEDOT:PSS/(AgNPS/SiNHS) and gold nanoparticles. It is possible to enhance the efficiency of solar cells by altering the surface of nanocomposite films made of AgNPS and SiNHS. Researchers found that films with metal nanoparticles had better optical absorption spectra over the full 600–850 nm wavelength range. Based on research on light absorption, half a weight percent of AuNPS is the optimal mass ratio. This was decided based on the findings of the investigations. Incorporating AuNPS into the PEDOT:PSS buffer layers and passivating the film surfaces increased the PCE from 4.8% to 6.1%. This allowed us to achieve our objective. As a result, there was a 27% improvement factor. Adding AuNPS to the devices also caused a substantial increase in the EQE value in the 600-1000 nm spectral range. Both the J sc and the FF were significantly increased after the application of the AuNPS. We attribute these findings mostly to the LSPR effects and enhanced light scattering of AgNPS. Together, these surface modification techniques and the incorporation of AuNPS into PEDOT:PSS buffer layers make for an excellent candidate for use in solar cells.

References

1. Zhu Y, Song T, Zhang F, Lee ST, Sun B (2013) Efficient organic-inorganic hybrid Schottky solar cell: the role of built-in potential. Appl Phys Lett 102(11):113504
2. Pudasaini PR, Sharma M, Ruiz-Zepeda F, Ayon AA (2014) Efficiency improvement of a nanostructured polymer solar cell employing atomic layer deposited Al_2O_3 as a passivation layer. Microelectron Eng 119:6–10

3. Zhang Y, Cui W, Zhu Y, Zu F, Liao L, Lee S-T, Sun B (2015) High efficiency hybrid PEDOT:PSS/nanostructured silicon Schottky junction solar cells by doping-free rear contact. Energy Environ Sci 8(1):297–302
4. Liu R, Lee S-T, Sun B (2014) 13.8% Efficiency hybrid Si/organic heterojunction solar cells with MoO_3 film as antireflection and inversion induced layer. Adv Mater 26(34):6007–6012
5. Zhang D, Jia R, Chen C, Ding W, Jin Z, Liu X, Ye T (2014) Reflectance and minority carrier lifetime of silicon nanoholes synthesized by chemical etching method. Chem Phys Lett 601:69–73
6. Han SE, Chen G (2010) Optical absorption enhancement in silicon nanohole arrays for solar photovoltaics. Nano Lett 10(3):1012–1015
7. Garnett E, Yang P (2010) Light trapping in silicon nanowire solar cells. Nano Lett 10(3):1082–1087
8. Yang TC, Huang TY, Lee HC, Lin TJ, Yen TJ (2011) Applying silicon nanoholes with excellent antireflection for enhancing photovoltaic performance. J Electrochem Soc 159(2): B104–B108
9. Hsiao YS, Charan S, Wu FY, Chien FC, Chu CW, Chen P, Chen FC (2012) Improving the light trapping efficiency of plasmonic polymer solar cells through photon management. J Phys Chem C 116(39):20731–20737
10. Liu K, Qu S, Zhang X, Tan F, Wang Z (2013) Improved photovoltaic performance of silicon nanowire/organic hybrid solar cells by incorporating silver nanoparticles. Nanoscale Res Lett 8(1):1–6
11. Kelly KL, Coronado E, Zhao LL, Schatz GC (2003) The optical properties of metal nanoparticles: the influence of size, shape, and dielectric environment. J Phys Chem B 107(3):668–677
12. Zayats AV, Smolyaninov II, Maradudin AA (2005) Nano-optics of surface plasmon polaritons. Phys Rep 408(3):131–314
13. Chen CH, Chen YF (1999) Strong and stable visible luminescence from Au-passivated porous silicon. Appl Phys Lett 75(17):2560-2562.
14. Snaith HJ, Moule AJ, Klein C, Meerholz K, Friend RH, Grätzel M (2007) Efficiency enhancements in solid-state hybrid solar cells via reduced charge recombination and increased light capture. Nano Lett 7(11):3372–3376
15. Yu P, Tsai CY, Chang JK, Lai CC, Chen PH, Lai YC, …, Wu CI (2013) 13% Efficiency hybrid organic/silicon-nanowire heterojunction solar cell via interface engineering. ACS Nano 7(12). 10780-10787