

PLASMONIC ENHANCED ORGANIC SOLAR CELLS

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PLASMONIC ENHANCED ORGANIC SOLAR CELLS

by

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CERTIFICATE

This is to certify that the thesis entitled “**PLASMONIC ENHANCED ORGANIC SOLAR CELLS**” being submitted by Kamal Kumar to Indian Institute of Technology Delhi for the award of the degree of **Doctor of Philosophy** is a record of bonafide research work carried out by him. He has worked under my guidance and supervision and has fulfilled the requirements, which to my knowledge have reached the requisite standard for the submission of the thesis. The results contained in this thesis have not been submitted in part or full to any other University or Institute for the award of any degree or diploma.

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ABSTRACT

In this thesis, the design and modeling of novel organic solar cells (OSCs) containing plasmonic nanostructures has been described such that the presence of the plasmonic nanostructures leads to an enhancement in the absorption in the active layer(s), the short circuit current density, as well as the efficiency of the solar cells. We investigate the effect of plasmonic nanostructures of different geometries and materials on the performance of single junction OSCs, double junction tandem OSCs, and triple junction tandem OSCs.

Firstly, a single junction organic solar cell (OSC) with plasmonic butterfly wing-shaped nanostructure embedded inside the active layer material (PTB7:PC₇₁BM) and ITO nano-grating on top has been proposed. Numerical modeling using Finite Difference Time Domain (FDTD) was employed to study the optical and electrical properties of the plasmonic OSC. Various parameters of the plasmonic nanostructure and the ITO grating were optimized to obtain a substantial enhancement of absorption in the active layer medium. The maximum values of absorption enhancement and power conversion efficiency (PCE) enhancement obtained using the optimized parameters of the nanostructures are ~20% and ~25%, respectively. The plasmonic butterfly wing-shaped nanostructures introduce in-plane light scattering which leads to an increased optical path length in the active layer. The addition of the ITO nano-grating on top enables light to be coupled and trapped into waveguide modes at the active layer.

A plasmonic double junction series connected tandem OSC, with PTB7:PC₇₀BM as the active layer material of the top subcell and PDPPSDTPS:PC₆₀BM as the active layer material of the bottom subcell, has also been proposed. This OSC, having Ag nanospheres over the top surface of the OSC and Ag nanostars within the active layer of the bottom subcell, has substantially enhanced absorption, short circuit current density (J_{sc}), and PCE as compared to a

reference tandem OSC that does not contain any nanoparticles. Different geometries of plasmonic nanoparticles – nanospheres and nanostars, were used to improve the absorption in different spectral regimes, corresponding to the absorption bands of the active layer materials of the two subcells. The effective J_{SC} of a series connected tandem solar cell is determined by the smaller J_{SC} of the subcells. The J_{SC} values of the two subcells were therefore matched by optimizing the thickness of the bottom subcell active layer, and by introducing plasmonic nanoparticles. A combination of plasmonic nanoparticles over the top surface and in the active layer bottom subcell results in high absorption and hence, higher J_{SC} . An overall J_{SC} enhancement of 26% was achieved by the manipulation of shape, size and surface coverage of Ag plasmonic nanoparticles in the different regions of the OSC. The tandem OSC containing the optimized Ag nanospheres over the top surface and Ag nanostars in the bottom subcell active layer has a calculated PCE of ~15.43%, compared to a maximum PCE of 12.25% in the reference tandem OSC without any nanoparticles.

We have also proposed the plasmonic enhancement of metal nanospheres added on a triple junction tandem organic solar cell. Gold, silver and aluminum nanospheres have individually optimized for size and surface coverage to boost the absorption in the OSC. Aluminum nanospheres of radius 70 nm and periodicity 350 nm is most effective in increasing the J_{SC} from the top and middle subcells and matching them to the J_{SC} from the bottom subcell. The resultant OSC with the optimized Al nanospheres has an open circuit voltage of 2.7 V and a short circuit current density of 9.61 mA/cm², leading to a calculated power conversion efficiency of 15.57%; an enhancement of 14% over the reference cell without the nanospheres.

Organic solar cell (OSC) containing plasmonic silver nanostructures in the active layer medium poly[[9-(1-octylnonyl)-9H-carbazole-2,7-diyl]-2,5-thiophenediyl-2,1,3-

benzothiadiazole-4,7-diyl-2,5-thiophenediyl] (PCDTBT):[6,6]-phenyl C71 butyric acid methyl ester (PC₇₁BM) were simulated using FDTD leading to a broadband enhancement in the absorption of the OSC. In this work, it was demonstrated that the enhancement was primarily because of the far-field scattering due to localized surface plasmon excitation from the nanostructures in the active layer. Geometries were optimized for plasmonic nanodiscs – of hexagon, square and circular cross-section. It was observed that the highest value of J_{SC} was obtained for hexagonal nanodiscs. An increase of 25.28% in the J_{SC} from the OSC containing hexagonal nanodiscs in the active medium was achieved.

Furthermore, FDTD is used to analyze the behavior of a plasmonics-enhanced organic solar cell (OSC) containing nanostructures of different plasmonic metals – gold, silver and aluminum, in the hole transport layer extending to the active layer of the solar cell. A low bandgap material – PDPPSDTPS:PC₆₀BM, was taken as the active layer material in this study. A comparison of the enhancement in the performance of organic solar cells (OSCs) — with respect to the absorption and J_{SC}, for circular nano-discs of different plasmonic metals introduced in the hole transport layer of the OSC was presented. A maximum J_{SC} of 22.72 mA/cm² was recorded for silver nano-discs having a radius of 100 nm, a surface coverage of 30% and height of 30 nm.

सार

इस थीसिस में, प्लास्मोनिक नैनोस्ट्रक्चर्स युक्त नये ऑर्गेनिक सोलर सेल्स (ओ एस सी) के डिजाइन और मॉडलिंग, जैसे कि प्लास्मोनिक नैनोस्ट्रक्चर की उपस्थिति के कारण सक्रिय परत (परतों) में अवशोषण में वृद्धि, लघु पथ धारा घनत्व में वृद्धि, साथ ही सोलर सेल की दक्षता में वृद्धि का वर्णन किया गया है। यहाँ हम विभिन्न ज्यामितीय और पदार्थों के प्लास्मोनिक नैनोस्ट्रक्चर के कारण एकल जंक्शन ऑर्गेनिक सोलर सेल्स, डबल जंक्शन टैंडम ऑर्गेनिक सोलर सेल्स, और ट्रिपल जंक्शन टैंडम ऑर्गेनिक सोलर सेल्स, के प्रदर्शन पर हुए प्रभाव की जांच करते हैं।

सबसे पहले, सक्रिय परत (पीटीबी७:पीसी७१बीएम) के अंदर उपस्थित प्लास्मोनिक तितली के पंखों के आकार वाले नैनोस्ट्रक्चर तथा शीर्ष पर आई टी ओ नैनो-ग्रेटिंग के साथ एक सिंगल जंक्शन ऑर्गेनिक सोलर सेल (ओ एस सी) प्रस्तावित किया गया है। इसमें ऑप्टिकल और विद्युत गुणों का अध्ययन करने के लिए संख्यात्मक मॉडलिंग परिमित अंतर समय डोमेन (एफ डी टी डी) को नियोजित किया गया है। सक्रिय परत में अवशोषण की पर्याप्त वृद्धि प्राप्त करने के लिए प्लास्मोनिक नैनोस्ट्रक्चर और आईटीओ नैनो-ग्रेटिंग के विभिन्न मापदंडों को अनुकूलित किया गया है। नैनोस्ट्रक्चर और आईटीओ नैनो-ग्रेटिंग के अनुकूलित मापदंडों का उपयोग करके अवशोषण वृद्धि और शक्ति रूपांतरण दक्षता में अधिकतम वृद्धि क्रमशः ~२०% और ~२५% प्राप्त की गई है। तितली पंखों के आकार का प्लास्मोनिक नैनोस्ट्रक्चर के कारण लाइट सक्रिय परत की सतह में बिखर जाती है जिसके कारण ऑप्टिकल पथ की लंबाई बढ़ जाती है। इसके अलावा शीर्ष पर आईटीओ नैनो-ग्रेटिंग प्रकाश को वेवगाइड मोड में युग्मित करके सक्रिय परत में फंसने में सक्षम बनाता है।

एक श्रृंखला में जुड़ा प्लास्मोनिक डबल जंक्शन टैंडम ऑर्गेनिक सोलर सेल (ओ एस सी), जिसमें ऊपर के सब-सेल में सक्रिय परत पदार्थ व नीचे के सब-सेल में सक्रिय परत पदार्थ क्रमशः पीटीबी७:पीसी७१बीएम व पीडीपीपीएसडीटीपीएस:पीसी६०बीएम के साथ भी प्रस्तावित है। इस आर्गेनिक सोलर सेल जिसमें ऊपर की सतह पर चाँदी के नैनोस्फियरस तथा निचली सक्रिय परत के भीतर चाँदी के नैनोस्टार लघु पथ धारा घनत्व तथा शक्ति रूपांतरण दक्षता में रिफ्रेन्स सोलर सेल की तुलना में काफी वर्द्धि हुई है।

ऐसा प्लास्मोनिक नैनोकणों के अलग-अलग ज्यामिति - नैनोस्फेर और नैनोस्टार्स, का उपयोग विभिन्न सब-सेल के सक्रिय परत सामग्री के अवशोषण बैंड के अनुरूप, विभिन्न वर्णक्रमीय क्षेत्रों में अवशोषण को बेहतर बनाने के लिए किया गया है। श्रृंखला से जुड़े टैंडेम सोलर सेल का प्रभावी लघु पथ धारा घनत्व दोनों सब-सेल में सबसे कम लघु पथ धारा घनत्व वाले सब-सेल द्वारा निर्धारित की जाती है। शीर्ष सतह पर और सक्रिय परत तल में प्लास्मोनिक नैनोकणों का एक संयोजन लघु पथ धारा घनत्व में उच्च अवशोषण में पैदा करता है। ओएससी के विभिन्न क्षेत्रों में चाँदी प्लास्मोनिक नैनोकणों के आकार, और सतह कवरेज के हेरफेर से 26% की कुल लघु पथ धारा घनत्व में वृद्धि हुई थी। टैंडेम आर्गेनिक सोलर सेल जिसमें ऊपरी सतह पर नैनोस्फियरस तथा निचली सक्रिय सतह में नैनोस्टार्स उपस्थित है, की पीसीड में रिफ्रेन्स सोलर सेल की तुलना में १५.४३% की वृद्धि हुई है।

हमने ट्रिपल जंक्शन टैंडेम आर्गेनिक सोलर सेल में जोड़े गए प्लास्मोनिक मेटल नैनोस्फेर के कारण सक्रिय परत में अवशोषण में वृद्धि का भी प्रस्ताव दिया है। ओएससी में अवशोषण को बढ़ाने के लिए अलग अलग आकार और सतह कवरेज के साथ सोने, चाँदी और एल्यूमीनियम नैनोस्फियर को ऊपरी सतह पर रखा गया है। शीर्ष और मध्य सब सेल की लघु पथ धारा घनत्व में अधिकतम वृद्धि के लिए ७० नैनो मीटर त्रिज्या तथा ३५० नैनो मीटर अंतराल के साथ एल्यूमीनियम नैनोस्फियर्स सबसे प्रभावी माना गया है। सोलर सेल की एल्यूमीनियम नैनोस्फियर्स साथ पीसीड १५.५७% प्राप्त की गई है। यह पीसीड रिफ्रेन्स सोलर सेल की पीसीड की तुलना में १४% अधिक है।

आर्गेनिक सोलर सेल जिसमें सक्रिय परत पीसीडीटीबीटी:पीसी७०बीएम में प्लास्मोनिक सिल्वर नैनोसंरचनाएं होती हैं, एफ डी टी डी का उपयोग करके अनुकरण किया गया था, जिससे ओ एस सी के अवशोषण में ब्रॉडबैंड वृद्धि हुई। इस कार्य में, यह प्रदर्शित किया गया है कि वृद्धि मुख्य रूप से सक्रिय परत में नैनोस्ट्रक्चर से स्थानीय सतह प्लैसमॉन उत्तेजना के कारण दूर-क्षेत्र के बिखरने के कारण हुई है। षट्कोण, वर्ग और वृत्त क्रॉस-सेक्शन के प्लास्मोनिक नैनोडिस्क के लिए ज्यामितीय अनुकूलित किया गया है। यह देखा गया कि जेएससी का उच्चतम वृद्धि षट्कोणीय नैनोडिस्क के लिए प्राप्त किया गया है। सक्रिय माध्यम में षट्कोणीय नैनोडिस्क युक्त ओएससी से जेएससी में 25.28% की वृद्धि हासिल की गई है।

इसके अलावा, एफ डी टी डी का उपयोग प्लास्मोनॉमिक्स-वर्धित कार्बनिक सौर सेल के व्यवहार का विश्लेषण करने के लिए किया जाता है, जिसमें विभिन्न प्लाज़्मोनिक धातुओं - सोना, चाँदी और एल्युमिनियम के नैनास्ट्रक्चर होते हैं, जो सौर सेल की सक्रिय परत में होते हैं। एक कम बैंडगैप कार्बनिक - पीडीपीपीएसडीटीपीएस:पीसी६०बीएम, को इस अध्ययन में सक्रिय परत सामग्री के रूप में लिया गया था। कार्बनिक सौर की सक्रिय परत में सिल्वर नैनो-डिस्क के लिए २२.७२ एमए/सीएम^{-२} का अधिकतम लघु पथ धारा घनत्व, १०० एनएम की त्रिज्या, ३०% की सतह कवरेज और ३० एनएम की ऊंचाई के लिए दर्ज किया गया था।

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CHAPTER 5

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– 50 nm, PTB7:PC₇₀BM layer – 170 nm, PDPPSDTPS:PC₆₀BM (i.e. LBG:PC₆₀BM) layer– 80 nm, TiO₂ layer – 50 nm, MoO₃ layer – 50 nm, and Ag back electrode – 100 nm. Top Ag nanosphere dimensions were taken to be: $R_T = 90$ nm, and $P_T = 500$ nm. Bottom Ag nanostar dimensions were taken to be: $r_B = 30$ nm, $L_B = 20$ nm, and $P_B = 250$ nm.119

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nanospheres in the top buffer layer (TiO₂) extending into the top subcell active layer and Ag nanostars in the bottom subcell (OSC J). The thicknesses of the different layers of the OSC were taken to be: ITO layer – 50 nm, PTB7:PC₇₀BM layer – 170 nm, PDPPSDTPS:PC₆₀BM (i.e. LBG:PC₆₀BM) layer – 80 nm, TiO₂ layer – 50 nm, MoO₃ layer – 50 nm, and Ag back electrode – 100 nm. Top Ag nanosphere dimensions were taken to be: R_T = 90 nm, and P_T = 500 nm. Bottom Ag nanostar dimensions were taken to be: r_B = 30 nm, L_B = 20 nm, and P_B = 250 nm.128

CHAPTER 6

Figure 6.1. (a) Schematic diagram of the triple junction tandem OSC with nanospheres over the top surface. (b) Schematic for OSC without nanospheres – the reference tandem OSC. The plane field monitors in the subcell active layers are shown – T₁ and T₂ are for the top subcell, M₁ and M₂ are for the middle subcell, and B₁ and B₂ are for the bottom subcell. The thicknesses of the layers of the OSCs were taken to be: ITO layer – 50 nm, TiO₂ layers – 10 nm, MoO₃ layers – 10 nm, and Ag Back Electrode – 100 nm.134

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Figure 6.5. Short circuit current density (J_{SC}) map for the variation of Al nanosphere radius ‘r’ and periodicity ‘P’ in the (a) top subcell, (b) middle subcell, and (c) bottom subcell of the tandem OSC with Al nanospheres over the top surface. The star marks the maximum subcell J_{SC} in each plot. (d) Absorption spectra of the top, middle and bottom subcells of the reference tandem OSC and the OSC containing Al nanospheres of radius, ‘r’ = 70 nm and

periodicity, ' P ' = 350 nm. The thicknesses of the different layers of the OSC were taken to be: ITO layer – 50nm , TiO₂ layer – 10 nm, MoO₃ layer – 10 nm, P3HT:PC₇₀BM layer – 150 nm, Si-PCPDTBT:PC₇₀BM layer – 150 nm, PMDPP3T:PC₇₀BM layer – 100 nm, and Ag back electrode – 100 nm.142

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CHAPTER 7

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