

DESIGN AND MODELING OF PLASMONIC ORGANIC SOLAR CELLS

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DESIGN AND MODELING OF PLASMONIC ORGANIC SOLAR CELLS

by

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CERTIFICATE

This is to certify that the thesis entitled “**DESIGN AND MODELLING OF PLASMONIC ORGANIC SOLAR CELLS**” being submitted by Pankaj Kumar Das 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

Photovoltaic technologies have the potential to become one of the world's major renewable energy sources in the future, provided they can meet rising global energy demands at much lower generating costs than traditional non-renewable energy sources. Initially, solar cell devices were based on silicon material, but these solar cells are prohibitively expensive because of the high material cost and its processing. Bulk heterojunction (BHJ) based organic solar cells (OSCs), which can be produced at a lower cost with earth-abundant materials and have long-term stability, have emerged as a potential candidate to replace high-priced silicon solar cells. The low power conversion efficiency of thin-film OSCs has become a major constraint in employing OSCs, which is mainly caused by insufficient light absorption of thin active layers. In order to increase the light absorption in the BHJ based thin-film active layer, several light trapping techniques have been introduced. The application of nanophotonics to thin-film OSCs is a great scientific approach which allows the possibility of shrinking the active layer (AL) thickness while maintaining the high levels of absorption in thin AL. This creates a great scope for new device structures i.e, plasmonic OSCs, which enable the manipulation and modeling of light in nanoscale dimensions.

The work presented in this thesis is primarily focused to design and modeling of OSCs comprising of an AL of low bandgap polymer containing plasmonic nanostructures in different regions of the solar cells such that the presence of the plasmonic nanostructures leads to an enhancement in the absorption in the AL, the short circuit current density, as well as the efficiency of the solar cells.

Firstly, a BHJ based OSCs comprising of low bandgap photoactive layers (PMDPP3T:PC70BM) with a 2-dimensional array of either Ag nano-spheres, nano-hemispheres,

or nano-parabolas embedded at the bottom of the cell has been proposed. Numerical modeling using Finite Difference Time Domain (FDTD) was employed to study and compare the photovoltaic properties of OSCs containing the different plasmonic nanostructures, in terms of optical absorption, short circuit current density (J_{SC}) and power conversion efficiency (PCE). Various geometrical parameters and period of the plasmonic nanostructures were optimized to obtain a substantial enhancement of light absorption in the AL. In this work, it was demonstrated that the single junction OSCs consisting of new AL polymer (PMDPP3T), blended with PC70BM can enhance the optical absorption in the visible and the NIR region. It was observed that the highest values of J_{SC} and PCE were obtained for optimized structure OSC having 2D arrays of Ag nano-parabolas at the back of the solar cell. An increase in J_{SC} and PCE of 26.41% and 26.37%, respectively, compared to a planar OSC was obtained for the OSC having a 2D array of parabolas at the bottom of the cell. The enhancement in photon absorption can be attributed due to the enhancement of light scattering from metallic nanostructures near their localized plasmon resonance.

BHJ-based OSCs comprising of low bandgap photoactive layers (PMDPP3T:PC70BM) and a combination of plasmonic nanostructures embedded in the cathode buffer layer and on top of the back Ag layer of OSCs have also been proposed. These OSCs having 2-dimensional (2D) arrays of Ag nanodiscs in the cathode buffer layer (CBL) in combination with 2D arrays of either Ag nanorings (Ag-NRs), Ag nanodiscs (Ag-NRs), or Ag hemispheres (Ag-HSs) at the back of the OSCs, have substantially enhanced absorption, short circuit current density (J_{SC}), and PCE as compared to a planar solar cell. FDTD simulations were performed to study and compare the photovoltaic characteristics of these OSCs having plasmonic nanostructures in different regions of the solar cells. Various geometrical parameters of plasmonic nanoparticles—nanodiscs, nanorings,

hemispheres, and periods were optimized to obtain a substantial light absorption enhancement in different spectral regimes, corresponding to the absorption bands of the AL materials. It was demonstrated that the OSC containing Ag-NDs in the CBL enhance the optical absorption in the lower and middle spectral regions. On the other hand, the integrated structure OSCs enhance the light absorption in the visible and NIR regions. A maximum enhancement in JSC and PCE of 40.36% and 40.36%, respectively, compared to a planar OSC was recorded for the OSC having an Ag-NDs array in the CBL in combination with an Ag-HSs array at the back of the cell.

Furthermore, this thesis also presents a comparative analysis of OSCs comprising of an AL of low and high bandgap polymers containing a combination of plasmonic nanostructures at the bottom of the cell and on the top of ITO. PTB7:PC71BM and PMDPP3T:PC70BM were taken as the AL material in this study. A combination of a 2D array of Ag nano-cubes at the bottom of the cell with a 2D array of either Ag nano-wires or Ag nano-cubes over the top surface of the OSC was employed to increase the optical absorption in the AL of OSCs. It was observed that the highest enhancement in J_{SC} and PCE of 37.27% and 37.26%, respectively, compared to a planar OSC was achieved for the OSC comprising of an AL of PMDPP3T:PC70BM having Ag nano-cubes array at the bottom of the cell in a combination with Ag nano-wires on top of the ITO of the OSC.

सार

फोटोवोल्टिक तकनीकों में भविष्य में दुनिया के प्रमुख नवीकरणीय ऊर्जा स्रोतों में से एक बनने की क्षमता है, बशर्ते वे पारंपरिक गैर-नवीकरणीय ऊर्जा स्रोतों की तुलना में बहुत कम उत्पादन लागत पर बढ़ती वैश्विक ऊर्जा मांगों को पूरा कर सकें। प्रारंभ में, सोलर सेल उपकरण सिलिकॉन सामग्री पर आधारित थे, लेकिन ये सोलर सेल महँगी सामग्री लागत और इसके प्रसंस्करण के कारण निषेधात्मक रूप से महँगी हैं। बल्क हेटेरोजंक्शन आधारित ऑर्गेनिक सोलर सेल, जो पृथ्वी पर प्रचुर मात्रा में पाए जाने वाले सामग्री के साथ कम लागत पर उत्पादित किया जा सकता है और इसकी दीर्घकालिक स्थिरता है, उच्च कीमत वाले सिलिकॉन सोलर सेल को बदलने के लिए एक संभावित उम्मीदवार के रूप में उभरा है। पतली-फिल्म वाली ऑर्गेनिक सोलर सेल की कम बिजली रूपांतरण दक्षता ऑर्गेनिक सोलर सेल को नियोजित करने में एक प्रमुख बाधा बन गई है, जो मुख्य रूप से पतली सक्रिय परतों के अपर्याप्त प्रकाश अवशोषण के कारण होती है। बल्क हेटेरोजंक्शन आधारित पतली-फिल्म सक्रिय परत में प्रकाश अवशोषण को बढ़ाने के लिए, कई प्रकाश फँसाने वाली तकनीकों को पेश किया गया है। पतली-फिल्म वाली ऑर्गेनिक सोलर सेल में नैनोफोटोनिक्स का अनुप्रयोग एक महान वैज्ञानिक दृष्टिकोण है जो पतली सक्रिय परत में प्रकाश अवशोषण के उच्च स्तर को बनाए रखते हुए सक्रिय परत की मोटाई को कम करने की संभावना को अनुमति देता है। यह नई डिवाइस संरचनाओं यानी, प्लास्मोनिक ऑर्गेनिक सोलर सेल के लिए एक महान गुंजाइश बनाता है, जो नैनोस्केल आयामों में प्रकाश के हेरफेर और मॉडलिंग की अनुमति देता है।

इस थीसिस में प्रस्तुत कार्य मुख्य रूप से प्लास्मोनिक नैनोस्ट्रक्चर युक्त पतली-फिल्म वाली ऑर्गेनिक सोलर सेल के डिजाइन और मॉडलिंग के लिए केंद्रित है, जैसे कि प्लास्मोनिक नैनोस्ट्रक्चर की उपस्थिति के कारण सक्रिय परत में अवशोषण में वृद्धि, लघुपथ धारा घनत्व में वृद्धि, साथ ही सोलर सेल की दक्षता में वृद्धि का वर्णन किया गया है।

सबसे पहले, बल्क हेटेरोजंक्शन आधारित कम बैंडगैप फोटोएक्टिव परत (PMDPP3T: PC70BM) वाले ऑर्गेनिक सोलर सेल जिसके निचले परत के ऊपर प्लास्मोनिक सिल्वर नैनो-स्फीयर, नैनो-हेमिस्फीयर, या नैनो-पैराबोला हैं उसको प्रस्तावित किया

गया है। प्रकाश अवशोषण, लघुपथ धारा घनत्व और बिजली रूपांतरण दक्षता के संदर्भ में, विभिन्न प्लास्मोनिक नैनोस्ट्रक्चर वाले ऑर्गेनिक सोलर सेल के फोटोवोल्टिक गुणों का अध्ययन और तुलना करने के लिए परिमित अंतर समय डोमेन (FDTD) का उपयोग करके संख्यात्मक मॉडलिंग को नियोजित किया गया है। सक्रिय परत में प्रकाश अवशोषण में पर्याप्त वृद्धि प्राप्त करने के लिए प्लास्मोनिक नैनोस्ट्रक्चर के विभिन्न ज्यामितीय मापदंडों और अवधियों को अनुकूलित किया गया है। इस कार्य में, यह प्रदर्शित किया गया कि PC70BM के साथ मिश्रित नए सक्रिय परत पॉलिमर PMDPP3T से युक्त एकल जंक्शन ऑर्गेनिक सोलर सेल विजिबल और नीयर इन्फ्रारेड क्षेत्र में ऑप्टिकल अवशोषण को बढ़ा सकते हैं। यह देखा गया कि सोलर सेल के निचले परत के ऊपर अनुकूलित संरचना के 2-आयामी सरणियों वाले प्लास्मोनिक सिल्वर नैनो-पैराबोला रखने से लघुपथ धारा घनत्व और बिजली रूपांतरण दक्षता में उच्चतम वृद्धि प्राप्त किए गए थे। सेल के निचले भाग में पैराबोला की 2-आयामी सरणी वाले ऑर्गेनिक सोलर के लिए समतल ऑर्गेनिक सोलर सेल की तुलना में लघुपथ धारा घनत्व और बिजली रूपांतरण दक्षता में क्रमशः 26.41% और 26.37% की वृद्धि प्राप्त की गई थी। फोटॉन अवशोषण में वृद्धि को उनके स्थानीयकृत प्लास्मोन नैनोस्ट्रक्चर से प्रकाश बिखरने में वृद्धि के कारण को जिम्मेदार ठहराया जा सकता है।

कम बैंडगैप फोटोएक्टिव परतों (पीएमडीपीपी3टी:पीसी70बीएम) से युक्त बल्क हेटेरोजंक्शन आधारित ऑर्गेनिक सोलर सेल जिसके कैथोड और इनोड बफर परत में प्लास्मोनिक नैनोस्ट्रक्चर का संयोजन है उसको प्रस्तावित किया गया है। इन ऑर्गेनिक सोलर सेल के कैथोड बफर परत में चांदी के नैनोडिस्क को रखा गया है, साथ ही सेल के सबसे निचले परत के ऊपर चांदी के नैनोरिंग्स, चांदी के नैनोडिस्क या चांदी के नैनो हेमीस्फियर को रखा गया है। यह देखा गया कि हाइब्रिड नैनोस्ट्रक्चर युक्त सोलर सेल की प्रकाश अवशोषण, लघुपथ धारा घनत्व और बिजली रूपांतरण छमता बगैर नैनोस्ट्रक्चर युक्त सोलर सेल के तुलना में बहुत अधिक है। विभिन्न प्लास्मोनिक नैनोस्ट्रक्चर वाले इन ऑर्गेनिक सोलर सेल की फोटोवोल्टिक विशेषताओं का अध्ययन और तुलना करने के लिए परिमित अंतर समय डोमेन (FDTD) सिमुलेशन किया गया है। सोलर सेल के सक्रिय परत (Active layer) के अवशोषण बैंड के अनुरूप विभिन्न स्पेक्ट्रल रेजिन में पर्याप्त प्रकाश अवशोषण वृद्धि प्राप्त करने के लिए प्लास्मोनिक नैनोस्ट्रक्चर जैसे कि

नैनोडिस्क, नैनोरिंग्स, और नैनो हेमीस्फीयर के विभिन्न ज्यामितीय मापदंडों और अवधियों (Periods) को ऑप्टिमाइज किया गया है। यह देखा गया कि कैथोड बफर परत में सिल्वर नैनोडिस्क युक्त ऑर्गेनिक सोलर सेल निचले और मध्य स्पेक्ट्रल रीजन में ऑप्टिकल अवशोषण को बढ़ाते हैं। दूसरी ओर, हाइब्रिड नैनोस्ट्रक्चर युक्त ऑर्गेनिक सोलर सेल विजिबल और नीयर इन्फ्रारेड क्षेत्रों में प्रकाश अवशोषण को बढ़ाते हैं। एक प्लैनर ऑर्गेनिक सोलर सेल की तुलना में ऑर्गेनिक सोलर सेल जिसके कैथोड बफर परत में चांदी के नैनोडिस्क है, साथ ही सेल के सबसे निचले परत के ऊपर चांदी के नैनो हेमीस्फीयर है उसके लघुपथ धारा घनत्व और बिजली रूपांतरण दक्षता में क्रमशः 40.36% और 40.36% की अधिकतम वृद्धि दर्ज की गई।

इसके अलावा, यह थीसिस ऑर्गेनिक सोलर सेल का एक तुलनात्मक विश्लेषण भी प्रस्तुत करती है जिसमें निम्न और उच्च बैंडगैप पॉलिमर की सक्रिय है तथा सेल के निचली परत के ऊपर और आईटीओ के शीर्ष पर प्लास्मोनिक नैनोस्ट्रक्चर का संयोजन है। इस अध्ययन में पीटीबी7:पीसी71बीएम और पीएमडीपीपी3टी:पीसी70बीएम को सक्रिय परत के रूप में लिया गया है। सेल के निचले भाग में सिल्वर नैनो-क्यूब्स के संयोजन के साथ या तो सिल्वर नैनो- वायर या सिल्वर नैनो-क्यूब्स को सोलर सेल के ऊपरी सतह पर रखा गया है ताकि ऑर्गेनिक सोलर सेल के सक्रिय परत में प्रकाश अवशोषण को बढ़ाया जा सके। यह देखा गया कि पीएमडीपीपी 3 टी: पीसी 70 बीएम की सक्रिय परत वाले ऑर्गेनिक सोलर सेल जिसके सबसे निचले परत के ऊपर चांदी के नैनो-क्यूब्स और सोलर सेल के सबसे ऊपरी परत के ऊपर नैनो- वायर रखा गया है उसके लघुपथ धारा घनत्व और बिजली रूपांतरण दक्षता में क्रमशः 37.27% और 37.26% की उच्चतम वृद्धि दर्ज की गई प्लैनर ऑर्गेनिक सोलर सेल की तुलना में।

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