On the physical and photo-electrical properties of organic photovoltaic cells based on 1,10 Phenanthroline and 10,15,20-tetra(4-pyridyl)-21H,23H-porphine non-fullerene thin films

Alina Irina (Radu) Calugar[1,2], Stefan Antohe [1,3]

[1]1University of Bucharest, Faculty of Physics, Research and Development Center for Materials and Electronic & Optoelectronic Devices (MDEO), Atomiștilor Street 405, 077125, Măgurele, Ilfov, Romania

[2]The National Institute for Laser, Plasma & Radiation Physics (INFLPR), Atomiștilor Street 409, 077125 Măgurele, Ilfov, Romania

[3]Academy of Romanian Scientists, Splaiul Independenței 54, 030167 Bucharest, Romania

alina.icalugar@yahoo.ro, santohe@solid.fizica.unibuc.ro

Abstract

The active layer of the bulk heterojunction organic photovoltaic cells is typically based on a polymeric blend containing a donor polymer and a fullerene-based polymer electron acceptor. However, in the last decade non-fullerene polymer-based solar cells have seen a rapid progress, due to their extraordinary chemical, thermal and photo stability, and because of their ability to decrease the voltage loss. The conventional Organic Photovoltaic Cells (OPVs), structures based on either P3HT:PCBM bulk heterojunction (BHJ) polymeric blend or P3HT/PCBM bilayer heterojunction, has limited efficiency and stability, in principal due to the fullerene derivatives used as acceptor component. PCBM for example, as many other fullerene derivatives, exhibits some deficiencies, such as: limited chemical and energetic tunability, small range of absorption spectra, morphological instability and relatively high production costs. That is why in the last years, novel non-fullerene materials started to be used in order to overcome the above limits associated with the fullerene acceptors. In this paper two different non-fullerene acceptor materials have been tested as potential candidates for the efficient OPVs based on P3HT donor polymer as main absorber: a new conjugated polymer containing chelating ligands like 1,10 Phenanthroline (Phen), and a small-molecule acceptor like 10,15,20-tetra(4-pyridyl)-21H,23H-porphine (TPyP). For both cell configurations a decrease of the voltage loss was obtained, and it was also observed that the thickness of the P3HT donor layer has an important contribution to the power output P_{max} and fill factor (FF) of the OPV structures.

Keywords: 1,10 Phenanthroline; Tetra(4-pyridyl)-21H,23H-porphine; Non-fullerene acceptors

Domain: physics

Section: Elaboration of the doctoral thesis

Motivation

One of the cheapest and most environmentally friendly source of renewable energy is the direct solar energy conversion by photovoltaic effect. The field of "Non-Fullerene" (NF) OPVs has been recently known a rapid development, reporting high performance NF-OPVs with obtained PCE values higher than 13-17% . One advantage of these NF-OPVs is the tunability of the energy offset between the donor and acceptor, hence reducing the voltage loss from the bandgap of the absorber to the open-circuit voltage (V_{OC}) of the cell with a relatively low driving force, but keeping a high short-circuit current (J_{SC}).

Methodology of Research

In this study, two types of OPVs have been fabricated, based on heterojunctions formed by P3HT as a donor and two non-fullerene organic thin films (Phen and TPyP) as acceptors. the proposed configurations have been particularly chosen, due to the favorable intrinsic energy band alignment of the selected materials. Effectively, the considered architectures comply with the "Fonash" model, where the HOMO energy levels favor the holes motion towards the "window"-electrode (ITO/Glass in

this case), whilst the LUMO energy levels facilitate the electrons transfer towards the metallic Al top-electrode. In this way, the performance losses given by a non-optimal charge transport through the OPV are expected to be reduced

Results and Comparison with State-of-the-art

In this work, together with the study of the behavior of these two NFAs in the OPVs based on P3HT donor polymer, we complementarily investigated the influence of the thickness of the P3HT donor layer on the OPVs performance, concluding that the thinner layers of P3HT could be more appropriate for reducing the series resistances, and thus improving further the fill factor (FF) of the OPV structures. The photovoltaic response exhibited a higher V_{OC} compared with the state-of-the-art conventional OPVs based on the "traditional" P3HT/PCBM heterojunction. It has been also pointed out that a thin layer of P3HT (smaller than $150\ nm$) is more appropriate to obtain bilayer OPV structures with a better FF and P_{max}.

Conclusions

The prepared OPV devices showed an enlarged action spectra as comparing with the action spectra of a single layer OPV structure having P3HT as main absorber. Although modest, the co-sensitization is present in the case of the prepared structures based on P3HT/Phen and P3HT/TPyP heterojunctions. These results open the new paths to the optimization of similar structures based on these cheap materials to improve their PCE.

Acknowledgements

The research work was supported by the Romanian Executive Unit for Financing Higher Education, Research, Development and Innovation (UEFISCDI) through the grants: 40PCCDI/2018, 33PCCDI/2018 and 18PCCDI/2018.

References

[1] K. Leo, Organic photovoltaics, Nature Reviews Materials 1 (2016) 16056. doi: 10.1038/natrevmats.2016.56.

[2] W. Zhao, S. Li, H. Yao, S. Zhang, Y. Zhang, B. Yang, J. Hou, Molecular Optimization Enables over 13% Efficiency in Organic Solar Cells, Journal of American Chemical Society 139 (2017) 7148−7151. doi: 10.1021/jacs.7b02677.

[3] C. J. Brabec, J. A. Hauch, P. Schilinsky, C. Waldauf, Production Aspects of Organic Photovoltaics and Their Impact on the Commercialization of Devices, MRS Bulletin (Materials Research Society) 30 (1) (2005) 50-52. doi: 10.1557/mrs2005.10.

[4] K. M. Coakley, M. D. McGehee, Conjugated Polymer Photovoltaic Cells, Chemistry of Materials (American Chemical Society) 16 (23) (2004) 4533-4542. doi: 10.1021/cm049654n.

[5] C. Locovei, D. Coman, A. Radu, L. Ion, V. A. Antohe, N. Vasile, A. Dumitru, S. Iftimie, S. Antohe, Physical properties of Cu and Dy co-doped ZnO thin films prepared by radio frequency magnetron sputtering for hybrid organic/inorganic electronic devices, Thin Solid Films 685 (2019) 379-384. doi: 10.1016/j.tsf.2019.06.027.

[6] B. Bita, S. Iftimie, A. Radu, V. A. Antohe, D. Coman, C. Miron, D. Staicu, L. Dan, L. Ion, S. Antohe, On the electrical and photo-electrical behavior of the photovoltaic cells based on polymeric and chlorophyll-a thin films, Proc. of the Romanian Academy – Series A 20 (1) (2019) 51-57.

[7] G. A. Nemnes, S. Iftimie, A. Palici, A. Nicolaev, T. L. Mitran, A. Radu, S. Antohe, Optimization of the structural configuration of ICBA/P3HT photovoltaic cells, Applied Surface Science 424 (2017) 264-268. doi: 10.1016/j.apsusc.2017.05.002.