

Advanced Materials for Photovoltaic Energy Harvesting

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Abstract

Design of novel materials is the key to ground breaking advancements in energy conversion. Solar radiation is a clean energy source with low environment impact but is still a difficult technology to be implemented on a large scale because of being an expensive technology. If global demands are to be met, new classes of solar cells with increased efficiency, reduced cost and new form factors must be developed. A lot of research is ongoing to find efficient materials which can supplement or supersede the existing silicon technology. In this review a general introduction covers the current scenario of energy demands of the world and where we stand in the search for alternative energy resources. A brief look into the working of photovoltaic systems and the conditions required to fabricate an ideal solar cell follows. Some of the advanced systems incorporated in solar cells over the past 20 years have been discussed along with their place in making photovoltaic technology efficient.

Keywords: Energy crisis, Photovoltaics, Organic semiconductor, Graphene, Thin-film technology.

1. Introduction

One of the most important challenges of this century is the quest to find alternative resources of energy to crude oil. Nobel laureate Richard Smalley listed 'Energy' as the first and foremost of

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humanity's problems for the next 50 years during one of his conference addresses. Energy is indeed a fundamental requirement in our everyday lives. There is legitimate evidence that fossil fuels are destined to end. The exact prediction of when it will end is questionable but the fact that it will end at some point leads to a plethora of uncertainty, fear and doubt over sustenance of life. The world-renowned geologist M. King Hubbert from Shell Oil Company presented a symmetric logistics distribution curve popularly referred to as the Hubbert curve (Fig 1) predicting the depletion of natural resources[1]. It is interesting to note that the peak-prediction (technically when half of the reserves have been exhausted) turned out to be quite accurate (1970). The steep decline in the resources as predicted by Hubbert necessarily means that there would not be enough time to cope with the exhaustion of existing fuel technologies and rise of equally efficient alternative technologies[1]. Thus, paving path for the future that increasingly includes non-conventional, clean, renewable and sustainable sources of energy is one of the most relevant research subject of the current times. Several carbon neutral energy sources have been harnessed over the past few decades like solar, wind, geothermal, biomass, hydroelectric power etc.

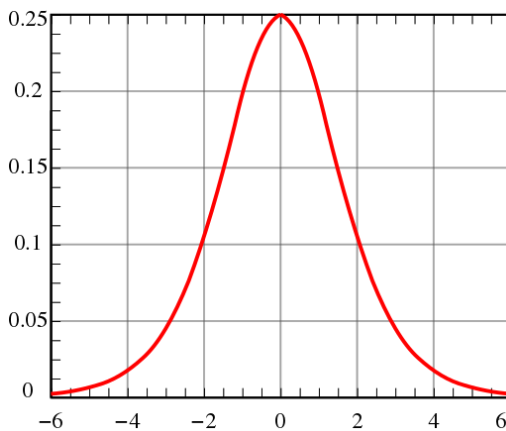


Figure: Hubbert curve - predicting the depletion of natural resources

Photovoltaic systems (solar cells) have been a very important alternative energy technology as a clean conversion of solar energy

into electricity. A photovoltaic device essentially consists of a semiconductor active layer sandwiched between electrodes[2]. Emergence of a photo voltage across the p-n junction in the semiconductor is the working principle in the arrangement. The active material in an ideal solar cell must possess a direct band structure with a band gap typically between 1.1 and 1.7 eV so that a good part of the solar spectrum is absorbed. The constituent materials must be readily available and non-toxic. The deposition techniques for device fabrication must be easily-reproducible and convenient for large area production[3]. The cell must also essentially exhibit good photovoltaic conversion efficiency, long-term stability and high light absorption coefficient. B and large photovoltaic conversion includes light harvesting, light absorption, excited state thermalization, energy diffusion, charge separation, charge transport and charge collection. Fig 2 shows the structural layout of a typical solar cell. The fabrication of a typical solar cell is as follows. A layer of Indium-Tin oxide is coated onto a glass substrate. This acts as a conductive and transparent electrode. A hole transport layer of PEDOT: PSS (poly(3,4-ethylenedioxythiophene) poly(styrene sulfonate)) is coated atop ITO to prevent leak currents and charge recombination[2]. The photoactive layer is a blend of the electron acceptor and donor atoms and the cathode interlayer is a low work-function metal used to lower the work function of the electrode on top to accept electrons.

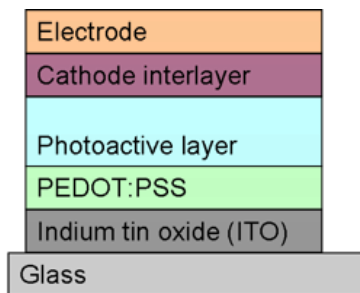


Figure: Structural layout of a bulk-heterojunction photovoltaic cell

Silicon has been the widely employed technology in highly efficient photovoltaics system. However, the high cost involved in the manufacturing makes it less desirable and alternative thin film

technologies are gaining popularity. In this review paper, I have made efforts to put together some of the recently developed advanced materials which can be integrated as active layers in thin-film photovoltaics, thereby providing cheaper, less toxic, easily processable photovoltaic cells with promising performance parameters.

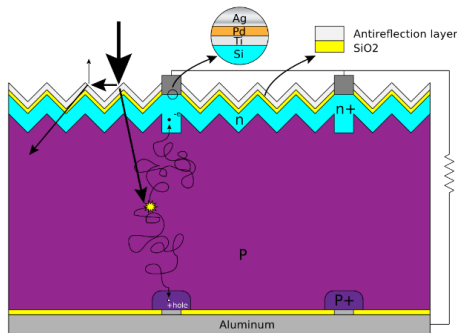


Figure 1: A typical Silicon solar cell structure

2. Graphene

Graphene is one of the best one atom thick, 2-D planar material with exceptional structural and electronic properties. The most interesting aspect is the ambipolar electric field effect which permits both electron and hole transport[4]. Graphene based materials have contributed to noteworthy enhancements in the efficiency of solar cells.

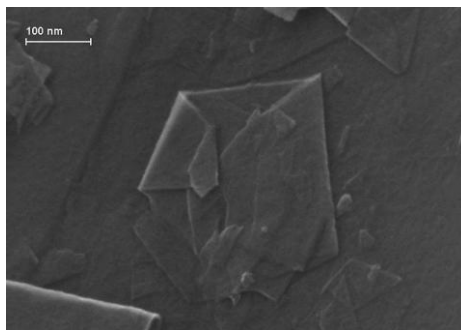


Figure 2: Graphene nanosheets as viewed under a scanning electron microscope

Graphene in semiconductor interface has been one of the foremost applications in photovoltaics. A graphene/titania interface was

shown to depict wavelength-dependant photocurrent generation and verified by ab-initio predictions[5]. Graphene has been investigated as an anchoring support for metal oxides and catalyst nanoparticles. This multifunctional designer system is an interesting perspective to be investigated in light conversion, fuel cells and photocatalysis. An aerosol mediated technique of decorating graphene with silver nanocrystals via non-covalent driving force, followed by migration and coalescence of the nanocrystals has also opened newer methods of investigating the interface fabrications for device performances[6].

Graphene based transparent electrodes can be fabricated by using spin coating. Graphene oxide sheets have been hybridized into silica sols using this technique[7]. Graphene films formed by exfoliation or thermally reduced graphene oxides can be employed as an electrode for dye-sensitized solar cells. An important feature exhibited by graphene-based electrodes is opening the path towards development of 'flexible technology'[8]. They are omnidirectionally stretchable with mechanical durability. Such electrodes have shown performance reliability under all types of deformations and can be significant in the route towards wearable integrated technology.

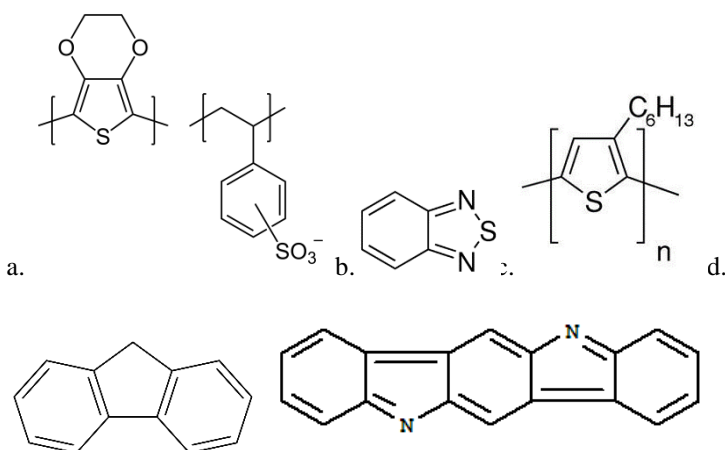


Figure 3: a. PEDOT:PSS; b. Benzothiadiazole; c. poly(3-hexylthiophene-2,5-diyl); d. Fluorene; e. Indolo(3,2)b-carbazole

PEDOT: PSS (Fig 5) is a commonly used hole transport material in photovoltaics. It is noteworthy that doping with graphene

enhances the hole mobility of PEDOT:PSS and this modified PEDOT:PSS has shown improved efficiency in perovskite based solar cells[9]. Graphene enabled enhanced hole transport. In organic solar cell built with poly(3-hexylthiophene-2,5-diyl) the recombination rate of electrons and holes was diminished with the inclusion of Graphene oxide nanosheets, establishing graphene oxide as an effective hole transport material[4].

3. Low bandgap polymers

Organic semiconductors are believed to be the foundation for cost-efficient solar energy conversion. This area of research has attracted numerous interests because of the high potential it holds in revolutionizing solar technology. Construction of low band gap polymers has been an active area of research to facilitate extension of absorption range of polymers well into the solar spectrum[10]. A copolymerized donor-acceptor structure has worked out to be the best in terms of achieving band gaps lower than 1.7 eV, so that the absorption maxima can be at 700 nm. The donor would be an electron rich moiety with a relatively higher HOMO energy level whereas the acceptor would be an electron deficient moiety with a lower LUMO energy level. When the two moieties are copolymerized there is an intramolecular charge transfer resulting in low band gap polymers[11].

2,1,3 Benzothiadiazole has received enormous attention as a molecular building block for organic semiconductor systems. It is an important class of luminescent compounds with strong electron withdrawing capacity thus making them useful as electron accepting materials[12]. Fluorene and its derivatives are another class of rigid, planar and stable molecules. They have unique photophysical properties and structural modifications are easier to facilitate tuning of the conjugation or to enhance the solubility. Selenium containing heterocycles have lower bandgaps than sulphur ones[13]. Indolo(3,2)b-carbazole polymers based materials are good hole transporters because of the aryl-amine type structure. It is an electron rich building block with excellent photostability and thermal stability. An important feature of low band gap polymers is the solubility. This is an important factor in determining the film-forming ability of the material. The charge

transfer properties are enhanced due to high mobility of the charge carriers. This along with purity and strong absorptions in near IR regions enables excellent harvesting of sunlight. [10].

4. Upconversion materials

Upconversion, otherwise known as ‘quantum-counter action’ is an anti-stokes emission that leads to the generation of one high energy photons for every two or more low energy photons. This is a non-linear optical process. Coupled lanthanide f ions when embedded in solid matrix deviate easily from stokes law leading to quantum counter action of anti-stokes emission types. Upconversion materials find application in solar cells to improve the overall performance. 52% of the total solar energy flux is in the IR region. Integration of Upconversion materials into the solar cell as a back layer to absorb the IR region of the solar radiation and reduce the sub band gap loss.

An important examples of the development of upconversion materials for photovoltaics is the one in GaAs solar cell, where a vitro-ceramic material with Er^{3+} and Yb^{3+} of roughly $100\ \mu\text{m}$ thickness was incorporated. Other examples include dye sensitized solar cells with $\text{LaF}_3:\text{Yb}/\text{Er}$ nanocrystals, bulk-heterojunction solar cells with $\text{P3HT}:\text{PCBM}:\text{LaF}_3:\text{Yb}/\text{Er}$, Er_2O_3 upconversion material combined with TiO_2 for photocatalytic application, $\text{ZnO}:\text{Cd}$ Tenanorod:quantum dot arrays and plasmon-enhanced $\text{NaYF}_4:\text{Yb}/\text{Er}$ nanoparticles[14]. The above quoted examples of upconversion nanomaterials in photovoltaic applications have been promising in enhancing the optical response of photovoltaic devices and photocatalysts to a wide solar spectrum. In spite of the benefits, efficient upconversion processes are observed to be limited to Er^{3+} , Tm^{3+} , and Ho^{3+} activators, distinguished by cascaded energy levels. Upconversion nanomaterials also require concentrated sunlight for effective output[15].

5. Conclusion and outlook

Solar cell technology is an ever-growing research area with novel materials and device configurations being researched and designed regularly. It is a promising alternative clean energy fuel with a lot

of potential to meet world energy demands and solve the impending energy crisis. Although photovoltaics have come a long way in terms of efficiency, stability and ease of fabrication, there are still a lot of avenues to be explored before it becomes ultimate and pivotal in energy harvesting. There is an impending need to design well-absorbing tuneable materials that are non-toxic and will also afford solution processable techniques of fabrication. Apart from the active layer designing and electrode modifications to enhance the efficiency and performance, another important key component is the encapsulant. Encapsulation is mandatory to ensure long-lasting performance and stability of the device. However, the epoxy resin which is the most popular encapsulant sometimes eats through the active layer and deteriorates the performance. Optimisation of the encapsulation process is therefore an interesting and demanding aspect of photovoltaics research. Flexible devices are another facet which can transform device appearances and also facilitate integration into textiles and lead to generation of wearable technology. Thus, with further research and insights photovoltaics will by all means turn into a more affordable, safe, cheaper and sustainable technology best suited for large scale use.

References

- [1] G.Ã. Maggio, G. Cacciola, "A variant of the Hubbert curve for world oil production forecasts", *Energy Policy*, vol. 37, 4761–4770, 2009. doi:10.1016/j.enpol.2009.06.053.
- [2] A. Goetzberger, C. Hebling, H. W. Schock, "Photovoltaic materials, history, status and outlook", *Mater. Sci. Eng. R Reports*, vol. 40, 1–46, 2003. doi:10.1016/S0927-796X(02)00092-X.
- [3] V.V. Tyagi, N.A.A. Rahim, N.A. Rahim, J.A., L. Selvaraj, "Progress in solar PV technology: Research and achievement", *Renew. Sustain. Energy Rev.*, vol. 20, 443–461, 2013. doi:10.1016/j.rser.2012.09.028.
- [4] G. Lu, S. Mao, S. Park, R.S. Ruoff, J. Chen, "Facile, Noncovalent Decoration of Graphene Oxide Sheets with Nanocrystals", 192–200, 2009. doi:10.1007/s12274-009-9017-8.
- [5] A. Du, Y.H. Ng, N.J. Bell, Z. Zhu, R. Amal, S.C. Smith, "Hybrid Graphene/Titania Nanocomposite: Interface Charge Transfer, Hole Doping, and Sensitization for Visible Light Response", 894–899, 2011. doi:10.1021/jz2002698.

- [6] P. V. Kamat, "Graphene-Based Nanoarchitectures. Anchoring Semiconductor and Metal Nanoparticles on a Two-Dimensional Carbon Support", 520-527, 2010. doi:10.1021/jz900265j.
- [7] S. Watcharotone, D.A. Dikin, S. Stankovich, R. Piner, I. Jung, G.H.B. Dommett, et al., "Graphene - Silica Composite Thin Films as Transparent Conductors", 2007.
- [8] X. Wang, L. Zhi, K. Mu, "Transparent, Conductive Graphene Electrodes for Dye-Sensitized Solar Cells", 2008. doi:10.1021/nl072838r.
- [9] J. Niu, D. Yang, X. Ren, Z. Yang, Y. Liu, X. Zhu, et al., "Graphene-oxide doped PEDOT: PSS as a superior hole transport material for high- efficiency perovskite solar cell", *Org. Electron.* 48 (2017) 165-171. doi:10.1016/j.orgel.2017.05.044.
- [10] E.B. Å, F.C. Krebs, "Low band gap polymers for organic photovoltaics", vol. 91, 954-985, 2007. doi:10.1016/j.solmat.2007.01.015.
- [11] T. Xu, L. Yu, "How to design low bandgap polymers for highly efficient organic solar cells", *Biochem. Pharmacol.* vol. 17 (11-15), 2014. doi:10.1016/j.mattod.2013.12.005.
- [12] J. Hou, H. Chen, S. Zhang, G. Li, Y. Yang, "Synthesis, Characterization, and Photovoltaic Properties of a Low Band Gap Polymer Based on Silole-Containing Polythiophenes" 16144-16145, 2008.
- [13] M.C. Scharber, N.S. Sariciftci, "Progress in Polymer Science Efficiency of bulk-heterojunction organic solar cells", *Prog. Polym. Sci.*, vol. 38 1929-1940, 2013. doi:10.1016/j.progpolymsci.2013.05.001.
- [14] J. Zhou, Q. Liu, W. Feng, Y. Sun, F. Li, "Upconversion Luminescent Materials : Advances and Applications", 2015. doi:10.1021/cr400478f.
- [15] C. Duan, L. Liang, L. Li, "Recent progress in upconversion luminescence nanomaterials for biomedical applications", 192-209, 2018. doi:10.1039/C7TB02527K.