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# High Efficient and Stable Solid Solar Cell: Based on $FeS_2$ nanocrystals and P3HT:PCBM

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**Abstract**

Nanocrystals(NCs)/polymer solid solar cells have the advantages of low-cost, simple process and flexible manufacturing. $FeS_2$ NCs is a kind of semiconductor with optical absorption in visible and near-infrared area, match well with the solar radiation spectrum. The solid solar cells based on $FeS_2$ NCs, poly(3-hexylthiophene) (P3HT) and phenyl-$C_{61}$-butyric acid methyl ester(PCBM), were prepared and achieved a photovoltaic conversion efficiency(*PCE*) of 3.0%. Besides, the device showed high stability with 83.3% of its initial efficiency remained after 15 weeks of exposure in air and stable performance in the range of 20-80°C. The *PCE* fluctuation magnitudes were also found smaller than quantum-dot sensitized solar cell (QDSSC) under the same condition.


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*Keywords*:$FeS_2$ nanocrystals; polymer; solar cell; PCE; stability

## 1.Introduction

Among varieties of renewable energy resources such as solar energy, wind energy, geothermal energy, biological energy, and nuclear energy, solar energy with excellent advantages of abundant source and non-pollution has become potential replacement of fossil fuels. Utilization of solar energy is aiming at converting light into electricity via photovoltaic device, like solar cell. Dating from 1954, Chapin et al successfully invented silicon solar cell with *PCE* of 6%[1], which is regarded as the first generation of solar cell. The copper indium gallium selenium (CuInGaSe) thin film solar cell, as the second generation of solar cell, was researched in early 1989s, with great breakthrough of *PCE* up to 13%[2]. However, the development of these two generations of solar cell have been restricted, since pure silicon is too much expensive and some elements (As, Cd) in  CuInGaSe thin film solar cell cause pollution issues. In recent

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years, new kinds of solar cells including dye-sensitized solar cell (DSSC) [3], QDSSC [4,5], polymer solar cell[6] and hybrid solar cell based on NCs and polymer[7-9], have been extensively investigated. DSSC and QDSSC with liquid electrolyte have poor stability, and slow electron transmission of polymer solar cell results in its low efficiency. Solar cell based on semiconductor NCs and polymer is one of promising alternatives to conventional silicon solar cell.

In NCs/polymer solid solar cell system, both semiconductor NCs and polymers act as sunlight absorbers and excitons generators. The polymer works as electron donor, while the semiconductor NCs works as acceptor. Moreover, the electron transmission in NCs is much faster than in polymers. As their absorption wavelength can be tuned according to size, composition and shape, NCs can be tuned to match the solar radiation spectrum. On the other hand, polymer materials have achieved great progress in stability. P3HT can overcome the disadvantage of previous materials such as polyurethane benzene phosphite vinyl(PPV), of which the branch chain is prone to oxidize decomposition under light illumination. Hence, the solid thin solar cell combines the strength of NCs and polymer, showing great potential in achieving high efficiency and stability.

During the past five years, Yuan et al [10-11 has obtained excellent results in fabrication of $FeS_2$ NCs via solvothermal reaction process and hydrothermal method. Pure and high quality $FeS_2$ NCs were facilely prepared and applied in solar cell. Compared with the typical NCs materials, including CdSe, CdTe, and CdS, $FeS_2$ NCs is not only nontoxic, but also has low band gap (about 1.0 eV), and compatibly high cost-performance.

## 2.Experimental

### *2.1.Materials and $FeS_2$ NCs preparation*

PCBM (99.5%) purchased from American Nano-C company and P3HT (90%) purchased from American Rieke metals company, were used as received. $FeS_2$ NCs was synthesized following the solvothermal reaction process described in literatures [10-11]. The obtained $FeS_2$ NCs was dispersed in chloroform and washed with excess of acetone, in order to remove organic impurities.

### *2.2.Active layer solution preparation*

The polymer active solution was prepared by dissolving 40 mg P3HT and 40 mg PCBM in 2 ml chlorobenzene. Subsequently, certain amounts of $FeS_2$ NCs were added to the solution, obtaining different concentrations (0, 1.25 mg/ml, 2.5 mg/ml, 3.75 mg/ml, 5 mg/ml, 6.25 mg/ml, 7.5 mg/ml) of $FeS_2$ NCs. The hybrid solutions were disposed by ultrasonic for more than 1 hour, obtaining uniformly dispersed solution before device fabrication.

### *2.3.Device fabrication*

In this paper, NCs/polymer solar cell was fabricated in inverted structure: FTO/$TiO_2$ layer/active layer ($FeS_2$:P3HT:PCBM)/PEDOT:PSS layer/Ag electrode, where $TiO_2$ and PEDOT:PSS act as electron selective layer and hole selective layer respectively, which are benefit for carriers transmission.

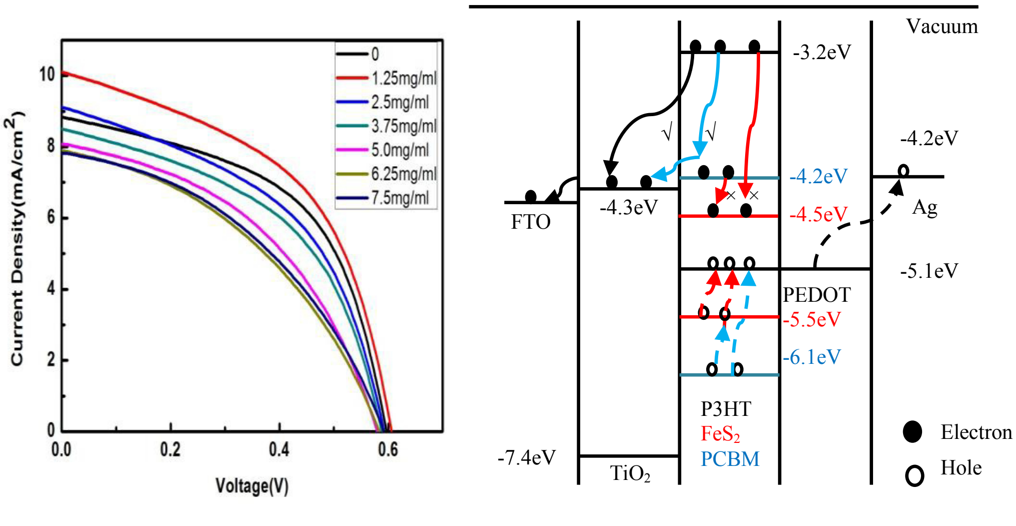
### *2.4.Characterization*

The current density versus voltage (*J-V*) characteristics of solar cell were measured with a solar simulator (ABET technology) under AM 1.5 (1000 W/m$^2$) irradiation intensity. The time stability of solar cell was conducted with continuous *J-V* measurement for 15 weeks. The thermal stability of solar cell was investigated by heating the devices to 20-80$^o$C, and the *J-V* characteristics were recorded. Besides, compared with the standard value (measured with irradiation intensity of 1000 W/m$^2$), the *PCE* fluctuation magnitudes were calculated with irradiation intensity changing from 500 W/m$^2$ to 2000 W/m$^2$.

## 3.Results and discussions

### *3.1.The effect of $FeS_2$ NCs in solid solar cell*

In Fig.1.(a), the *J-V* characteristics of fabricated solar cells with different concentrations of $FeS_2$ were compared. The open voltage($V_{oc}$) of all devices were close to 0.6 V, and an obvious enhancement of current density ($J_{sc}$) was observed with the $FeS_2$ NCs concentration of 1.25 mg/ml. The detailed values were listed in Table 1.




(a) (b)

Fig.1.(a) *J-V* characteristics of fabricated solar cells with different concentrations of $FeS_2$
(b) Schematic diagram of the energy levels in the $FeS_2$ NCs / polymer solar cells

Table1. Photovoltaic parameters of fabricated solid solar cells with different concentrations of $FeS_2$.

| Concentration(mg/ml) | $J_{sc}$(mA/cm$^2$) | $V_{oc}$(V) | *FF*(%) | *PCE*(%) |
|---|---|---|---|---|
| 0 | 8.84 | 0.61 | 51.9 | 2.8 |
| 1.25 | 10.11 | 0.60 | 50.2 | 3.0 |
| 2.5 | 9.12 | 0.59 | 47.6 | 2.6 |
| 3.75 | 8.51 | 0.59 | 48.5 | 2.4 |
| 5 | 8.10 | 0.58 | 44.3 | 2.1 |
| 6.25 | 7.91 | 0.58 | 40.7 | 1.9 |
| 7.5 | 7.84 | 0.59 | 41.5 | 1.9 |

According to the results of concentrations of 0 and 1.25 mg/ml, the addition of $FeS_2$ NCs can increase $J_{sc}$ from 8.84 mA/cm$^2$ to 10.11 mA/cm$^2$, resulting an increased *PCE* from 2.8% to 3.0%. This was attributed to the improvement of light harvesting capability of $FeS_2$ NCs in solar cell. However, when the concentrations increased from 2.5 mg/ml to 7.5 mg/ml , $J_{sc}$ showed a trend of decrease, where fill factor(*FF*) and *PCE* presented the same trend. This problem was ascribed to the structure of energy levels in solar cell, as shown in Fig.1.(b).

Upon incidence of irradiation, both polymer and $FeS_2$ NCs absorb photons and generate excitons. The excitons separate at the donor-acceptor interfaces. As shown in Fig.1.(b), electrons can be transferred from P3HT to $TiO_2$ (the black curve), PCBM (the blue curve), and $FeS_2$ (the red curve). The hole transportation is accomplished inversely. However, as the LUMO value of $FeS_2$ (-4.5 eV) is lower than that of $TiO_2$(-4.2 eV), the electrons which is transferred to $FeS_2$ can't reach $TiO_2$ layer, resulting in less efficient electrons collection. When the solid solar cell incorporated less $FeS_2$ NCs (like 1.25 mg/ml), the advantages of $FeS_2$ near-infrared absorption and rapid transmission carriers were greater than its defects in electronic transmission, so the $FeS_2$ NCs/polymer solar cell displayed better performance than polymer solar cell. On the condition that the concentration of $FeS_2$ NCs in solar cell became higher, the defects were more obvious than its advantages, resulting in a large numbers of electrons fail of transfering, thus $J_{sc}$ gradually decreased and so *PCE* declined. This is the reason why solid solar cell based on $FeS_2$ NCs and polymer had optimized efficiency at a certain concentration of $FeS_2$.

### *3.2. Time stability and thermal stability of $FeS_2$ NCs/polymer solar cell*

Taking the fabricated solar cells with $FeS_2$ concentration of 1.25 mg/ml for example, both time stability and thermal stability of NCs / polymer solar cells were investigated. As shown in Table 2, with a *J-V* measurement lasting for 15 weeks, $J_{sc}$ gradually decreased from 10.11 mA/cm$^2$ to 8.19 mA/cm$^2$, and *PCE* from 3.0% to 2.5%. As a result, 83.3% of its original efficiency was remained. Although Zhong et al had reported a high *PCE* of QDSSC[4], the liquid electrolyte system had a common and severe problem of leakage, resulting a short working life of QDSSC as 22 days[4]. Comparably, solid solar cell shows better time stability.

Tabel 2. The photovoltaic parameters of $FeS_2$ NCs/polymer solar cell at different duration time

| Duration time(week) | $J_{sc}$(mA/cm$^2$) | $V_{oc}$(V) | *FF*(%) | *PCE*(%) |
|---|---|---|---|---|
| 0 | 10.11 | 0.60 | 50.2 | 3.0 |
| 1 | 9.66 | 0.60 | 50.3 | 2.9 |
| 2 | 9.28 | 0.59 | 48.8 | 2.7 |
| 3 | 8.84 | 0.60 | 53.1 | 2.8 |
| 5 | 8.71 | 0.60 | 52.4 | 2.7 |
| 7 | 8.56 | 0.59 | 52.5 | 2.7 |
| 10 | 8.45 | 0.59 | 52.5 | 2.6 |
| 15 | 8.19 | 0.60 | 50.6 | 2.5 |

Moreover, the thermal stability in range of 20-80$^o$C was investigated and compared, as shown in Fig.2. $J_{sc}$, $V_{oc}$, *FF* and *PCE* of $FeS_2$ NCs/polymer solar cell almost kept the same value; while those of QDSSC displayed a sharp decline. Also because of its liquid electrolyte system, QDSSC was more suitable between 20$^o$C and 40$^o$C, while $FeS_2$ NCs/polymer solar cell showed wider working temperature range (20-80$^o$C) with stable performance.

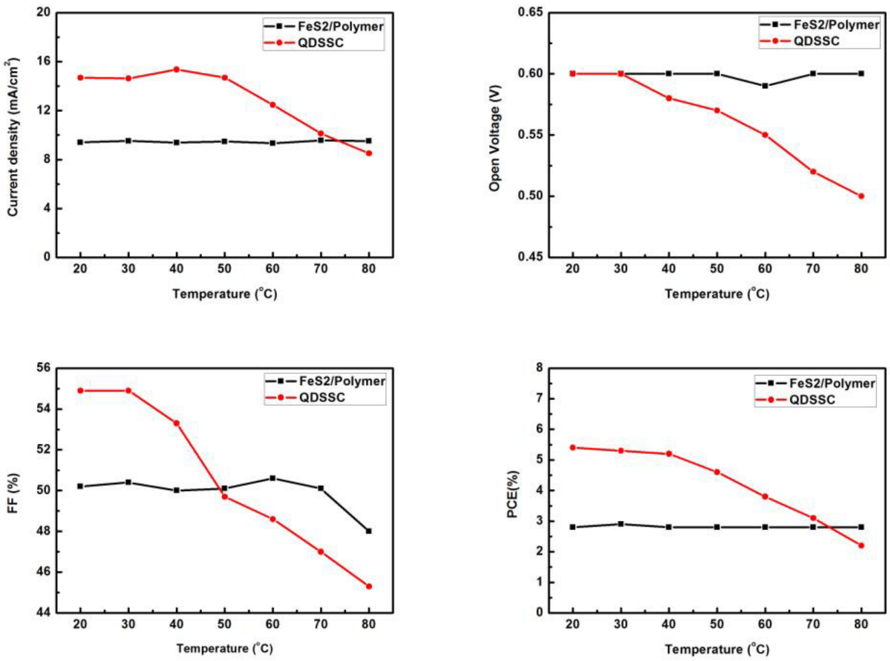



Fig.2.Thermal stability comparison of $FeS_2$ NCs/polymer solar cell and QDSSC.

### *3.3. PCE fluctuation of fabricated solar cells under different irradiation intensity*

It is well known that the irradiation intensity of the same location on the ground is constantly changing during the daytime. Generally, the standard irradiation intensity is 1000 $W/m^2$, and a corresponding *PCE*($\eta_{1000}$) is regarded as the standard value. In this paper, the influence of irradiation intensity tuning from 500 $W/m^2$ to 2000 $W/m^2$ was investigated. The device could absorb more light and generate more excitons with the light intensity increasing. This was the reason why *PCE* was proportional to intensity (as shown in Table 3). Meanwhile, the *PCE* fluctuation magnitudes (α) of fabricated solar cell had been calculated and compared with QDSSC. Both in strong and weak irradiation intensity, the *PCE* fluctuation magnitudes of QDSSC(26.4%, -22.6%)were larger than $FeS_2$ NCs / polymer solar cells(±20.8%).

Table 3. Comparison of $FeS_2$ NCs/polymer solar cells and QDSSC in *PCE* fluctuation magnitudes

| Intensity | $FeS_2$ NCs/polymer solar cell | | QDSSC | |
|---|---|---|---|---|
| （$W/m^2$） | *PCE*(%) | $\alpha=100\%(\eta-\eta_{1000})/\eta_{1000}$ | *PCE*(%) | $\alpha=100\%(\eta-\eta_{1000})/\eta_{1000}$ |
| 500 | 1.9 | -20.8% | 4.1 | -22.6% |
| 800 | 2.2 | -8.3% | 4.8 | -9.4% |
| 1000 | 2.4 | 0 | 5.3 | 0 |
| 1200 | 2.5 | 4.2% | 5.8 | 9.4% |
| 1500 | 2.7 | 12.5% | 6.3 | 18.9% |
| 2000 | 2.9 | 20.8% | 6.7 | 26.4% |

## 4.Conclusion

The solid solar cells based on $FeS_2$ NCs and P3HT:PCBM were fabricated in inverted structure. Due to the addition of $FeS_2$ NCs into polymer solar cells, an enhanced light harvest was achieved, resulting an obvious increase of $J_{sc}$, while too much $FeS_2$ NCs brought the defects of electron transmission loss. The solid solar cell achieved its optimal *PCE* of 3.0% at $FeS_2$ concentration of 1.25 mg/ml. The fabricated solar cells were proven to be of high stability, with 83.3% of its initial efficiency remained after 15weeks of exposure in air and quite stable performance between 20$^{o}$C and 80$^{o}$C. Furtherly, the *PCE* fluctuation magnitudes were smaller than that of QDSSC under the same condition.

## Acknowledgements

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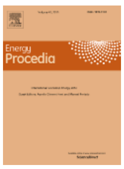

**Biography**

**Weiling Luan** received her doctorate in material science and technology in 1998 at Shanghai Institute of Ceramics, CAS. Then she was a postdoctoral researcher at Utsunomiya University in Japan. Now, she is a professor at East China University of Science and Technology. Her research interest includes micro chem.-mechanical system and sustainable energy.