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Letter

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Enhanced efficiency of flexible GaN/perovskite solar cells based on piezo-phototronic effect

Yuru Wang [1, †], Dongqi Zheng [1, †], Lijie Li [2, *], and Yan Zhang [1,3, *]

[1] *School of Physics, School of Electronic Science and Engineering, University of Electronic Science and Technology of China, Chengdu 610054, China*

[2] *Multidisciplinary Nanotechnology Centre, College of Engineering, Swansea University, Swansea, SA1 8EN, UK*

[3] *Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing 100083, China; College of Nanoscience and Technology, University of Chinese Academy of Sciences, Beijing 100049, China*

[†] These authors contributed equally to this work.

[*] To whom correspondence should be addressed, E-mail: L.Li@swansea.ac.uk and zhangyan@uestc.edu.cn

Abstract

Solar cells fabricated by piezoelectric semiconductor materials, such as GaN, AlN and CdS, enable better performance due to the piezo-phototronic modulation. Recent experiments have revealed the possibility to further improve the energy conversion efficiency of perovskite solar cells with a gallium nitride (GaN) substrate as the electron transport layer. In this study, a perovskite piezo-phototronic solar cell with a GaN layer has been investigated theoretically. The open-circuit voltage, current-voltage curves, fill factor, efficiency of power conversion, and power of maximum output under applied strains are obtained. While the applied strain is 1%, the open-circuit voltage has been improved by 3.8%. This design can offer a practical approach to produce high-efficiency perovskite solar cells.

Keywords

Piezotronic; Piezo-phototronic; solar cells; perovskite solar cell; GaN

1. Introduction

Piezoelectric semiconductor materials, such as GaN, AlN and CdS, have attracted tremendous attention in the field of nano-science [1]. Based on the coupling of piezoelectric and semiconductor properties, these novel materials have been applied in various electronic and optoelectronic devices such as nanogenerators [2-4] ,piezoelectric field effect transistors [5-8], piezotronic light emitting diodes [9] and piezo-phototronic solar cells [10]. Solar cells fabricated by piezoelectric semiconductor materials enabled a better performance based on the piezo-phototronic effect [4, 11-13].

Since the first report of efficient solid perovskite cells was published in 2012, there has been a rapid growth in research and development of perovskite solar cells due to their superior properties, including high solar absorption, low carrier recombination and effortless fabrication [14-17]. Recent advances also revealed the piezo-phototronic characteristics of perovskite materials and proposed a design of peizo-phototronic effect enhanced perovskite solar cell [18]. Meanwhile, recently conducted experiments have revealed the possibility to further improve the energy conversion efficiency in the graded bandgap perovskite solar cell with a GaN substrate as the electron transport layer [19].

The basic principle of a solar cell is that the built-in electric field separates electron-hole pairs generated by incidenting photons in a metal-semiconductor contact or a p-n junction. Piezoelectric field induced by piezoelectric charges can efficiently improve the separation process of photo-generated electron-hole pairs [4, 20]. Such photovaltic devices, called piezo-phototronic solar cell (PSC) have been fabricated experimentally [21-23]. A high energy conversion efficiency has been essential for large-scale photovoltaic systems [24]. The perovskite solar cells with the GaN substrate can have potential to achieve high conversion efficiencies. There are several noteworthy semiconductor properties of GaN PSC. The piezoelectric constant (0.73 C/m^2) of GaN is large [25], and the relative dielectric constant (8.9) is small [26], which gives rise to realization of extraordinary piezoelectrical adjustments. Meanwhile, the graded bandgap perovskite solar system also shows excellent performance with the short-circuit current density of 42.1 A/cm^2 and the fill factor of ~75%, which paves the way for the high performance GaN perovskite PSC.

This work describes a perovskite piezo-phototronic solar cell with a GaN layer, with improved performance by applying the piezo-phototronic effect [19]. Fig.1 schematically shows the structure of the design. The structure is considered as a multi-junction solar cell. The main structure is a GaN layer sandwiched between the top electrode material and the perovskite layer, as illustrated in Fig. 1(a) [22]. The top electrode material together with the GaN layer can form a p-n or a metal semiconductor (m-s) junction [22]. The GaN layer serves as an electron transferring layer in perovskite solar cells, the potential barrier at GaN/perovskite interface can be neglected [27]. For the top electrode material-GaN junction, the p-n or m-s model can be used for simulating the piezo-phototronic properties. The piezoelectric charges can accumulate at the interface between the top layer and the GaN layer, where the depletion region is formed, which is for generating the built-in potential and adjust the transportation process of photon-generated carriers. The piezoelectric charges will screen at the GaN/perovskite interface due to the good conductivity of GaN and perovskite, and there is no potential barrier and depletion region in the GaN/perovskite contact [1, 28]. Fig.1 (b) and (c) show that the piezoelectric filed formed by accumulated charges enhances or reduces the Schottky barrier, respectively. Piezoelectric field is able to assist the separation of electron-hole pairs in the p-n or m-s contact by increasing the built-in potential. The characteristic parameters to evaluate the performance of solar cells, i.e. open-circuit voltage (V_{oc}), current-voltage characteristics, fill factor (FF), power conversion efficiency (PCE), and maximum output power (P_m), are studied in this work. The open-circuit voltage of the perovskite solar cell with a GaN layer increases by 3.8%, and the ratio to quantify the piezo-phototronic modulation is simulated for PSCs. Piezoelectric potential will enhance the built-in electric filed which can improve the separation and transportation of electron-hole pairs. Therefore, the electrical current increases under applied strains [27-28]. Further detailed research of this effect will be discussed in our future work. The principle of the piezo-phototronic solar cell is able to offer a practical method to produce an integrated photovoltaic system with higher efficiency and lower cost.

2. Piezo-phototronic modulation on GaN-based solar cells

The characteristics of PSC are elucidated by piezo-phototronic theoraticl model. V_{oc} of the PSC increases when an external strain is applied on the device and piezoelectric charges are induced. The theoretical models are built for p-n junction solar cells, and similar theoretical analysis can be obtained in metal-semiconductor solar cells [29]. The total current density of the p-n junction solar cell is given by [27]:

$$J = J_{pn}\left[\exp\left(\frac{qV}{kT}\right)-1\right]-J_{solar} \tag{1}$$

Here J_{pn} is the saturation current, J_{solar} denotes the short-circuit current density, k stands for the Boltzmann constant, T represents the temperature, q is the elementary charge and V is the applied voltage. The saturation current can be obtained by [27]:

$$J_{pn} = \frac{qD_p p_{n0}}{L_p}+\frac{qD_n n_{p0}}{L_n} \tag{2}$$

Where D_p is hole diffusion constant and D_n is electron diffusion constant. L_p is hole diffusion length and L_n is electron diffusion. And p_{n0} is the thermal equilibrium holes concentration in the n-type semiconductor, n_{p0} is the thermal equilibrium electrons concentration in the p-type semiconductor, and $p_{n0} = n_i\exp\left(\frac{E_i - E_{Fn}}{kT}\right)$, $n_{p0} = n_i\exp\left(\frac{E_{Fp} - E_i}{kT}\right)$, where n_i is the intrinsic carrier denstity, E_i is the intrinsic Fermi level, and E_{Fn} and E_{Fp} are the Fermi levels of the n-type and p-type semicondutors respectively. So the saturation current density J_{pn0} without piezopotential can be expressed as [27]:

$$J_{pn0} = \frac{qD_p n_i}{L_p}\exp\left(\frac{E_i - E_{Fn0}}{kT}\right)+\frac{qD_n n_i}{L_n}\exp\left(\frac{E_{Fp0} - E_i}{kT}\right) \tag{3}$$

where E_{Fn0} and E_{Fp0} are the Fermi levels of the n-type and p-type semicondutors in the absence of piezopotential respectively. Based on the theory of piezo-phototronic solar cells, the Fermi level E_{Fn} of n-type semiconductor and the Fermi level of p-type semiconductor E_{Fp} in the presence of piezopotential can be obtained by [28]:

$$E_{Fn} = E_{Fn0} - \frac{q^2 \rho_{piezo} W^2{}_{piezo}}{2\varepsilon_s} \tag{4}$$

$$E_{Fp} = E_{Fp0} + \frac{q^2 \rho_{piezo} W^2{}_{piezo}}{2\varepsilon_s} \tag{5}$$

where ρ_{piezo} denotes the piezoelectric charge density, W_{piezo} symbolizes the piezoelectrically generated charges distribution width, ε_s is the dielectric constant. Substituting Equation (2-5) into Equation (1), the current-voltage characteristics of the piezoelectric p-n junction solar cell can be given by:

$$J = \left(\frac{qD_p p_{n0}}{L_p} + \frac{qD_n n_{p0}}{L_n} \right) \exp\left(\frac{q^2 \rho_{piezo} W^2{}_{piezo}}{2\varepsilon_s kT} \right) \left[\exp\left(\frac{qV}{kT} \right) - 1 \right] - J_{solar} \tag{6}$$

The induced piezoelectric charges within the GaN layer can be expressed as [4]:

$$q\rho_{piezo} W_{piezo} = -e_{33}\varepsilon \tag{7}$$

Where e_{33} is piezoelectric constant in *c*-axis, and ε is the applied strain.

V_{oc} can be obtained as:

$$V_{oc} \approx \frac{kT}{q} \left[\ln\left(\frac{J_{solar}}{J_{pn}} \right) + \frac{q^2 \rho_{piezo} W^2{}_{piezo}}{2\varepsilon_s kT} \right] \tag{8}$$

The scale ratio γ can represent the piezo-phototronic modulation for the PSC in terms of the open-circuit voltage and other output performances, derived with the method reported in [18], which is

$$\gamma = \frac{\dfrac{q^2 \rho_{piezo} W^2{}_{piezo}}{2\varepsilon_s kT}}{\ln\left(\dfrac{J_{solar}}{J_{pn}} \right)} \tag{9}$$

Furthermore, the output power is derived to

$$P(V) = VJ(V) = V \left\{ J_{pn} \exp\left(\frac{q^2 \rho_{piezo} W^2{}_{piezo}}{2\varepsilon_s kT} \right) \left[\exp\left(\frac{qV}{kT} \right) - 1 \right] - J_{solar} \right\} \tag{10}$$

When the power is at the maximum, the voltage satisfies the following equation:

$$V_m + \frac{kT}{q} \ln\left(\frac{qV_m}{kT} + 1 \right) = \frac{kT}{q} \left[\ln\left(\frac{J_{solar}}{J_{pn}} \right) + \frac{q^2 \rho_{piezo} W^2{}_{piezo}}{2\varepsilon_s kT} \right] \tag{11}$$

Consequently, V_m varies with the piezoelectric charges induced by the ε. The maximum power current density can be obtained as:

$$J_m = \left(\frac{qD_p p_{n0}}{L_p} + \frac{qD_n n_{p0}}{L_n} \right) \exp\left(\frac{q^2 \rho_{piezo} W^2{}_{piezo}}{2\varepsilon_s kT} \right) \left[\exp\left(\frac{qV_m}{kT} \right) - 1 \right] - J_{solar} \tag{12}$$

Thus, the maximum output power P_m can be calculated by:

$$P_m = V_m J_m \tag{13}$$

The fill factor can be derived from the method described in reference [18],

$$FF = \frac{P_m}{J_{solar} V_{oc}} = \frac{J_m V_m}{J_{solar} V_{oc}} \tag{14}$$

The power conversion efficiency (PCE) is defined in [18]:

$$PCE = \frac{J_{solar} V_{oc} FF}{P_{in}} \tag{15}$$

3. Results and discussions

Typical constants are used in calculations of the V_{oc}, P_m, PCE, and FF. The temperature has been designated at 300K, W_{piezo} is assumed to be 0.543 nm [30], the relative dielectric constant of GaN is 8.9 [26], and e_{33} of the GaN has the value of 0.73 C/m^2 [25].

Fig. 2(a) is the schematic of the model for simulation. A GaN layer is sandwiched between the top material and the perovskite layer. The relative current density J/J_{pn0} versus voltage (J/J_{pn0}-V curve) of the GaN PSC with the external strain varying in the range of [-1% 1%] when the J_{solar} is 42.1 mA/cm^2 [19] is plotted in Fig. 2(b). Fig. 2(c) displays the curve of P versus V, indicating that the J rises with the strain and reaches a maximum value at V_m. By calculating the Eq. (3) and Eq. (8), the V_{oc} linearly relating to the strain ε, together with the relation between P_m and the ε, are displayed in the Fig. 2(d). By introducing the piezo-phototronic effect, the properties of the GaN PSC improve due to the enhancement of V_m and P_m.

The modulation ratio γ for PSC as the function of W_{piezo} and the ε is plotted in Fig. 3 (a). As W_{piezo} varies in the region of 48 – 55 nm, corresponding to strain of -1.0% (compressive) and strain of 1.0% (tensile), the γ changes from -3.232 % to 3.703 %. Fig. 3(b) is the γ versus the strain when J_{solar} is at 42.1 mA/cm^2 [19] and 0.83 mA/cm^2 [31]. As the W_{piezo} widens, the γ increases, as illustrated in Fig. 3(c). Both the semicondutor and the top material can influence the W_{piezo} [32-33]. Fig. 3(d) depicts the ratio γ relating to the applied strain for three piezoelectric materials: GaN, CdS and AlN. The ratio γ is calculated by using the same parameters of GaN (J_{sc}, J_{pn0}, etc.) except for the piezoelectric constant and the relative dielectric constant. The piezoelectric constants are 0.73 C/m^2 (GaN) [25], 0.44 C/m^2 (CdS) [34-35], 1.46 C/m^2 (AlN) [36]. The relative dielectric constants are 8.9 (GaN) [26], 5.7 (CdS) [37], 9.14 (AlN) [38]. Fig. 3(d) displays that the curve of CdS is close to GaN's, and the ratio γ of AlN increases more distinctly than GaN's and CdS's with the strain varying from -1% to 1%. When considering the influence of material properties, the ratio of piezoelectric constant to relative dielectric constant plays an important role in the performance of PSC. Using the Eqs. (9) and (10), FF and PCE, properties describing the characteristics of PSCs, are presented in Fig. 4(a) and Fig. 4(b) with the ε increasing linearly in the region of [-1% 1%]. A better output performance of the GaN PSC is demonstrated attributed to the improved *FF* and *PCE* caused by increasing V_{oc} with the applied external strain.

Piezophototronic effects of other 8 types of piezoelectrical materials have been calculated and summarised in Table 1. The PCE, FF, V_{oc} and γ of PSC based on different materials are calculated with different e_{33} and ε_r under a strain of 1% respectively, and other parameters concerned with calculations, such as J_{sc}, J_{pn0} and etc, are the same as precedent calculations of GaN solar cell. As shown in Table 1, the ratio γ of AlN is about two times larger than GaN's. The preferable performances of AlN, GaN and CdS are benefited from large piezoelectrical constants and small relative dielectric constants, indicating that a better performance may be obtained from the material whose piezoelectrical constant is large and relative dielectric constant is small. The two-dimensional electron gas mobility in the GaN can be enhanced because the piezoelectric effect is able to improve electron confinement described in a previous literature [39], as well as conductivity of GaN, which is a function of the electron mobility [27].

4. Conclusion

To conclude, the concept of piezotronically enhanced GaN perovskite PSC has been postulated and subsequently simulated in this work. Key parameters characterizing the device including V_{oc}, P_m, P, and FF have been mathematically calculated. It is shown that the PSC demonstates improved performances under externally applied strains, especially for the open-circuit voltage. Moreover, GaN and AlN show a greater potential for high-efficiency PSCs than other piezoelectric materials. The simulation results provide physical insights of the GaN perovskite PSCs and can serve as guidance on the design of perovskite piezo-phototronic energy harvesting devices.

Figure caption

Fig.1. Schematic of the structure and the energy band diagram of the GaN and perovskite PSC. (a) without strain. (b) with the tensile strain. (c) with the compressive strain. The color variance depicts the schematic of the piezopotential at the GaN layer.

Fig. 2. (a) Conceptual diagram of a GaN PSC based on p-n junction (upper side) and Ohmic contact (bottom side). (b). Relative current density-voltage (J/J_{pn0}-V -V) curve with ε increasing in the range of [-1% 1%]. (c) The output power of a GaN PSC as function of

voltage as ε is within the region of [-1% 1%]. (d) P_m and V_{oc} versus the external strain applied.

Fig. 3. (a) γ of PSC changes with W_{piezo} and the external strain. (b) γ of the GaN PSC versus the ε. (c) γ of the GaN PSC in relation to W_{piezo} under the ε of 0.2% to 1% with a step size of 0.4%. (d) The γ of the simulated device versus the strain ε with three piezoelectric materials: GaN, CdS and AlN.

Fig.4. (a) *FF* and (b) *PCE* of GaN PSC with the applied strain varying in the region [-1% 1%].

Table:

Table 1. Comparison between the performances of piezoelectric solar cells based on 9 types of materials.

Materials	e_{33}(C/m^2)	ε_r	PCE	FF	V_{oc}(V)	γ
CdTe	0.03[36]	11[40]	24.48%	84.40%	0.689	0.12%
CdSe	0.347[35]	5.8[41]	25.18%	84.69%	0.706	2.67%
CdS	0.440[35]	5.7[37]	25.40%	84.77%	0.711	3.44%
InP	0.04[36]	12.5[42]	24.48%	84.40%	0.689	0.14%
InAs	-0.03[36]	15.15[42]	24.47%	84.39%	0.689	0.08%
InN	0.97[36]	15.3[26]	25.23%	84.70%	0.707	2.83%
GaN	0.73[25]	8.9[26]	25.46%	84.79%	0.713	3.66%
AlN	1.46[36]	9.14[38]	26.42%	85.16%	0.734	7.12%
GaAs	-0.12[36]	13[40]	24.56%	84.43%	0.691	0.41%

(PCE, V_{oc}, FF of Table 1 are calculated under 1% strain, and PCE, V_{oc}, FF are 21.7%, 0.688V, 0.75).

Reference

1. Wang, Z. L., Piezotronics and Piezo-phototronics. *Nature Reviews Materials* **2016,** *1* (34), 23-24.

2. Wang, X.; Song, J.; Liu, J.; Wang, Z. L., Direct Current Nanogenerator Driven by Ultrasonic Wave, Science, 316: 102-105. *Science* **2007,** *316* (5821), 102-105.

3. Water, W.; Fang, T. H.; Ji, L. W.; Lee, C. C., Effect of growth temperature on photoluminescence and piezoelectric characteristics of ZnO nanowires. *Materials Science & Engineering B* **2009,** *158* (1), 75-78.

4. Zhang, Y.; Yang, Y.; Wang, Z. L., Piezo-phototronics effect on nano/microwire solar cells.

Energy & Environmental Science **2012,** *5* (5), 6850-6856.

5. Wu, W.; Wei, Y.; Wang, Z. L., Strain-gated piezotronic logic nanodevices. *Advanced Materials* **2010,** *22* (42), 4711.

6. Gao, S.; Wang, Y.; Wang, R.; Wu, W., Piezotronic effect in 1D van der Waals solid of elemental tellurium nanobelt for smart adaptive electronics. *Semiconductor Science Technology* **2017,** *32* (10).

7. Wu, W.; Wang, L.; Li, Y.; Zhang, F.; Lin, L.; Niu, S.; Chenet, D.; Zhang, X.; Hao, Y.; Heinz, T. F., Piezoelectricity of single-atomic-layer MoS2 for energy conversion and piezotronics. *Nature* **2014,** *514* (7523), 470-474.

8. Wu, W.; Wen, X.; Wang, Z. L., Taxel-addressable matrix of vertical-nanowire piezotronic transistors for active and adaptive tactile imaging. *Science* **2013,** *340* (6135), 952-7.

9. Yang, Q.; Wang, W.; Xu, S.; Wang, Z. L., Enhancing light emission of ZnO microwire-based diodes by piezo-phototronic effect. *Nano Letters* **2011,** *11* (9), 4012-4017.

10. Hu, Y.; Zhang, Y.; Chang, Y.; Snyder, R. L.; Wang, Z. L., Optimizing the power output of a ZnO photocell by piezopotential. *Acs Nano* **2010,** *4* (7), 4220.

11. Wang, Z. L., Piezopotential gated nanowire devices: Piezotronics and piezo-phototronics. *Nano Today* **2010,** *5* (6), 540-552.

12. Wang, Z. L.; Wu, W., Piezotronics and piezo-phototronics: fundamentals and applications. *National Science Review* **2014,** *1* (1), 62-90.

13. Wu, W.; Wang, Z. L., Piezotronics and piezo-phototronics for adaptive electronics and optoelectronics. *Nature Reviews Materials* **2012,** *24* (34), 23-24.

14. Green, M. A.; Ho-Baillie, A.; Snaith, H. J., The emergence of perovskite solar cells. *Nature*

Photonics **2014,** *8* (7), 506-514.

15. Yang, Y.; You, J., Make perovskite solar cells stable. *Nature* **2017,** *544* (7649), 155-156.

16. Albrecht, S.; Rech, B., Perovskite solar cells: On top of commercial photovoltaics. *Nature Energy* **2017,** *2* (1), 16196.

17. Huang, J.; Yuan, Y.; Shao, Y.; Yan, Y., Understanding the physical properties of hybrid perovskites for photovoltaic applications. *Nature Reviews Materials* **2017,** *2* (7), 17042.

18. Gu, K.; Zheng, D.; Li, L.; Zhang, Y., High-efficiency and stable piezo-phototronic organic perovskite solar cell. *Rsc Advances* **2018,** *8* (16), 8694-8698.

19. Ergen, O.; Gilbert, S. M.; Pham, T.; Turner, S. J.; Tan, M. T. Z.; Worsley, M. A.; Zettl, A., Graded bandgap perovskite solar cells. *Nat Mater* **2017,** *16* (5), 522-525.

20. Pan, C.; Chen, M.; Yu, R.; Yang, Q.; Hu, Y.; Zhang, Y.; Wang, Z. L., Progress in Piezo-Phototronic - Effect - Enhanced Light - Emitting Diodes and Pressure Imaging. *Advanced Materials* **2016,** *28* (8), 1535.

21. Jiang, C.; Jing, L.; Huang, X.; Liu, M.; Du, C.; Liu, T.; Pu, X.; Hu, W.; Wang, Z. L., Enhanced Solar Cell Conversion Efficiency of InGaN/GaN Multiple Quantum Wells by Piezo-Phototronic Effect. *Acs Nano* **2017,** *11* (9).

22. Wen, X.; Wu, W.; Wang, Z. L., Effective piezo-phototronic enhancement of solar cell performance by tuning material properties. *Nano Energy* **2013,** *2* (6), 1093-1100.

23. Zhu, L.; Wang, L.; Pan, C.; Chen, L.; Fei, X.; Chen, B.; Yang, L.; Li, S.; Zhong, L. W., Enhancing the Efficiency of Silicon-Based Solar Cells by the Piezo-Phototronic Effect. *Acs Nano* **2017,** *11* (2), 1894-1900.

24. Polman, A.; Knight, M.; Garnett, E. C.; Ehrler, B.; Sinke, W. C., Photovoltaic materials:

Present efficiencies and future challenges. *Science* **2016,** *352* (6283), aad4424.

25. Wan, S.-p.; Xia, J.-b.; Chang, K., Effects of piezoelectricity and spontaneous polarization on electronic and optical properties of wurtzite III–V nitride quantum wells. *Journal of Applied Physics* **2001,** *90* (12), 6210-6216.

26. Levinshteĭn, M. E.; Rumyantsev, S. L.; Shur, M., *Properties of advanced semiconductor materials : GaN, AlN, InN, BN, SiC, SiGe*. John Wiley: 2001.

27. Sze, S. M., *The physics of semiconductor devices*. Oxford University Press: 1979; p 34.

28. Zhang, Y.; Liu, Y.; Wang, Z. L., Fundamental theory of piezotronics. *Adv Mater* **2011,** *23* (27), 3004-13.

29. Zheng, D. Q.; Zhao, Z.; Huang, R.; Nie, J.; Li, L.; Zhang, Y., High-performance Piezo-phototronic Solar Cell Based on Two-dimensional Materials. *Nano Energy* **2017,** *32*, 448-453.

30. Liu, W.; Zhang, A.; Zhang, Y.; Wang, Z. L., Density functional studies on wurtzite piezotronic transistors: influence of different semiconductors and metals on piezoelectric charge distribution and Schottky barrier. *Nanotechnology* **2016,** *27* (20), 205204.

31. Matioli, E.; Neufeld, C.; Iza, M.; Cruz, S. C.; Al-Heji, A. A.; Chen, X.; Farrell, R. M.; Keller, S.; DenBaars, S.; Mishra, U.; Nakamura, S.; Speck, J.; Weisbuch, C., High internal and external quantum efficiency InGaN/GaN solar cells. *Applied Physics Letters* **2011,** *98* (2), 021102.

32. Suvansinpan, N.; Hussain, F.; Zhang, G.; Chiu, C. H.; Cai, Y.; Zhang, Y. W., Substitutionally doped phosphorene: electronic properties and gas sensing. *Nanotechnology* **2016,** *27* (6), 065708.

33. Zhang, Y.; Liu, W.; Wang, Z. L., First principle simulations of piezotronic transistors. *Nano Energy* **2015,** *14*, 355-363.

34. Arlt, G.; Quadflieg, P., Piezoelectricity in iii-v compounds with a phenomenological analysis of the piezoelectric effect. *Physica Status Solidi* **1968,** *25* (1), 323-330.

35. Berlincourt, D.; Jaffe, H.; Shiozawa, L. R., Electroelastic Properties of the Sulfides, Selenides, and Tellurides of Zinc and Cadmium. *Physical Review* **1963,** *129* (3), 1009-1017.

36. Bernardini, F.; Fiorentini, V.; Vanderbilt, D., Spontaneous polarization and piezoelectric constants of III-V nitrides. **1997,** *56* (16), 10024-10027.

37. Lippens, P. E.; Lannoo, M., Calculation of the band gap for small CdS and ZnS crystallites. *Physical Review B Condensed Matter* **1989,** *39* (15), 10935.

38. Collins, A. T.; Lightowlers, E. C.; Dean, P. J., Lattice Vibration Spectra of Aluminum Nitride. *Physical Review* **1967,** *158* (3), 833-838.

39. Maeda, N.; Saitoh, T.; Tsubaki, K.; Nishida, T.; Kobayashi, N., Enhanced Electron Mobility in AlGaN/InGaN/AlGaN Double-Heterostructures by Piezoelectric Effect. *Japanese Journal of Applied Physics* **1999,** *38* (Part 2, No. 7B), L799-L801.

40. Strzalkowski, I.; Joshi, S.; Crowell, C. R., Dielectric constant and its temperature dependence for GaAs, CdTe, and ZnSe. *Applied Physics Letters* **1976,** *28* (6), 350-352.

41. Wakaoka, T.; Hirai, K.; Murayama, K.; Takano, Y.; Takagi, H.; Furukawa, S.; Kitagawa, S., Confined synthesis of CdSe quantum dots in the pores of metal-organic frameworks. *Journal of Materials Chemistry C* **2014,** *2* (35), 7173-7175.

42. Zhang, Y.; Nie, J.; Li, L., Piezotronic effect on the luminescence of quantum dots for micro/nano-newton force measurement. *Nano Research* **2017**.

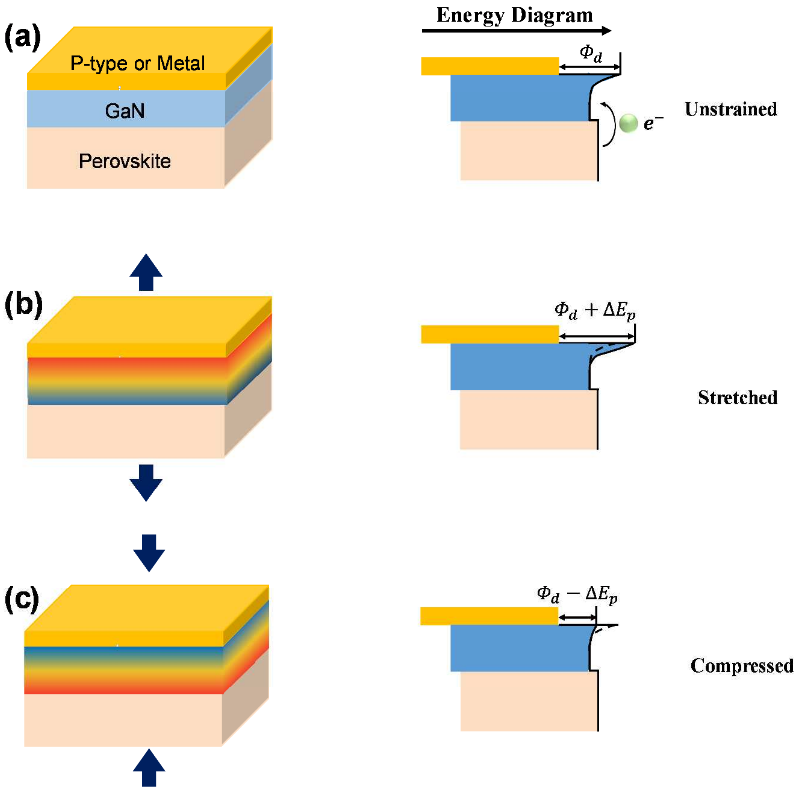
(a)
P-type or Metal
GaN
Perovskite
Energy Diagram
Φ_d
e^-
Unstrained
(b)
$\Phi_d + \Delta E_p$
Stretched
(c)
$\Phi_d - \Delta E_p$
Compressed

Figure 1

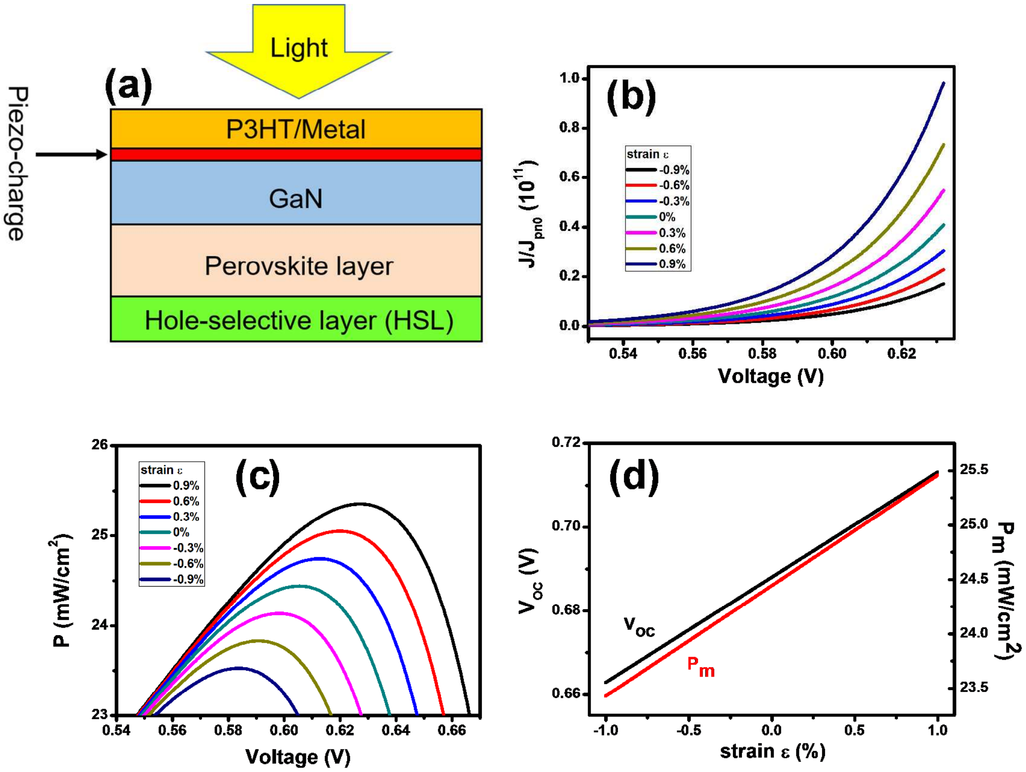
Light
(a)
Piezo-charge
P3HT/Metal
GaN
Perovskite layer
Hole-selective layer (HSL)
(b)
J/J$_{pn0}$ (10^{11})
strain ε
-0.9%
-0.6%
-0.3%
0%
0.3%
0.6%
0.9%
Voltage (V)
(c)
P (mW/cm^2)
strain ε
0.9%
0.6%
0.3%
0%
-0.3%
-0.6%
-0.9%
Voltage (V)
(d)
V$_{OC}$ (V)
V$_{OC}$
P$_m$
P$_m$ (mW/cm^2)
strain ε (%)

Figure 2

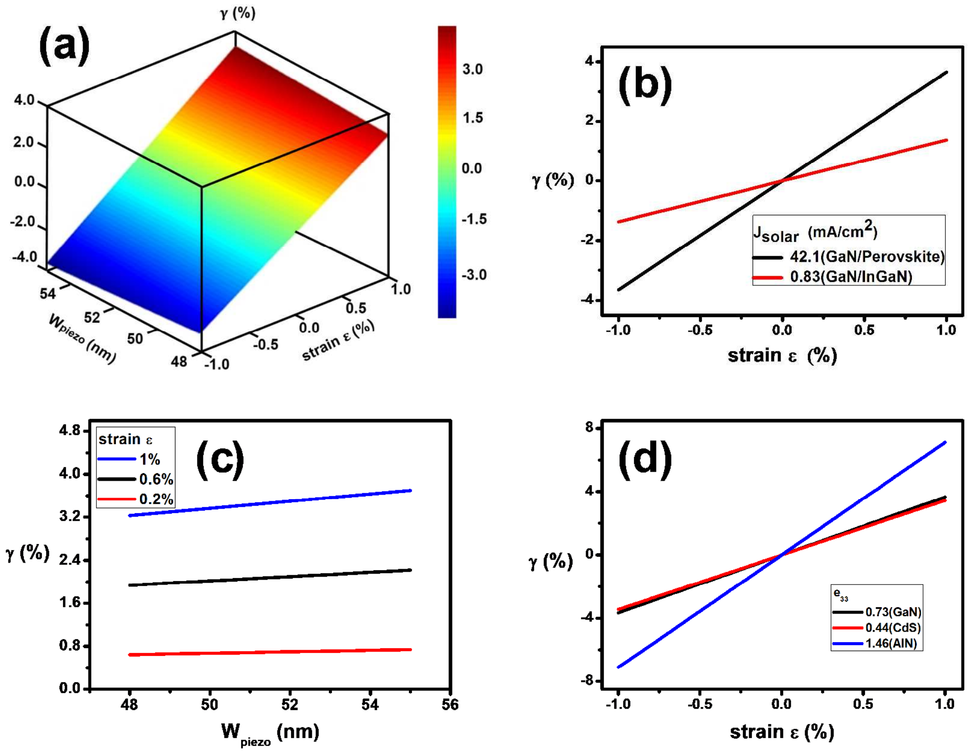
(a)
γ (%)
4.0
2.0
0.0
-2.0
-4.0
54
52
50
48
Wpiezo (nm)
-1.0
-0.5
0.0
0.5
1.0
strain ε (%)
3.0
1.5
0.0
-1.5
-3.0
(b)
γ (%)
4
2
0
-2
-4
Jsolar (mA/cm2)
42.1(GaN/Perovskite)
0.83(GaN/InGaN)
-1.0
-0.5
0.0
0.5
1.0
strain ε (%)
(c)
strain ε
1%
0.6%
0.2%
γ (%)
4.8
4.0
3.2
2.4
1.6
0.8
0.0
48
50
52
54
56
Wpiezo (nm)
(d)
γ (%)
8
4
0
-4
-8
e33
0.73(GaN)
0.44(CdS)
1.46(AlN)
-1.0
-0.5
0.0
0.5
1.0
strain ε (%)

Figure 3

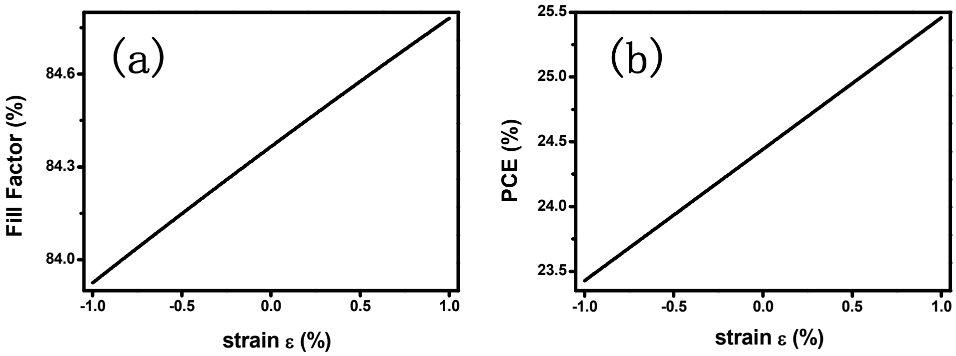
(a)
Fill Factor (%)
84.6
84.3
84.0
-1.0
-0.5
0.0
0.5
1.0
strain ε (%)
(b)
PCE (%)
25.5
25.0
24.5
24.0
23.5
-1.0
-0.5
0.0
0.5
1.0
strain ε (%)

Figure 4

Enhanced efficiency of flexible GaN/perovskite solar cells based on piezo-phototronic effect

Yuru Wang [1, †], Dongqi Zheng [1, †], Lijie Li [2, *], and Yan Zhang [1,3, *]

[1] *School of Physics, School of Electronic Science and Engineering, University of Electronic Science and Technology of China, Chengdu 610054, China*

[2] *Multidisciplinary Nanotechnology Centre, College of Engineering, Swansea University, Swansea, SA1 8EN, UK*

[3] *Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, Beijing 100083, China; College of Nanoscience and Technology, University of Chinese Academy of Sciences, Beijing 100049, China*

[†] These authors contributed equally to this work.

[*] To whom correspondence should be addressed, E-mail: L.Li@swansea.ac.uk and zhangyan@uestc.edu.cn