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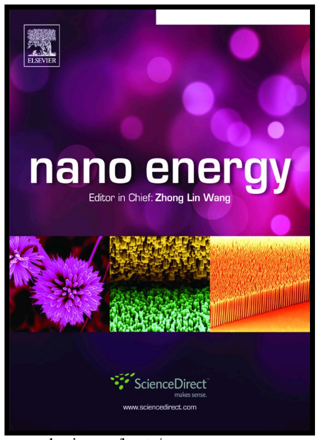

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High-performance Piezo-phototronic Solar Cell Based on Two-dimensional Materials

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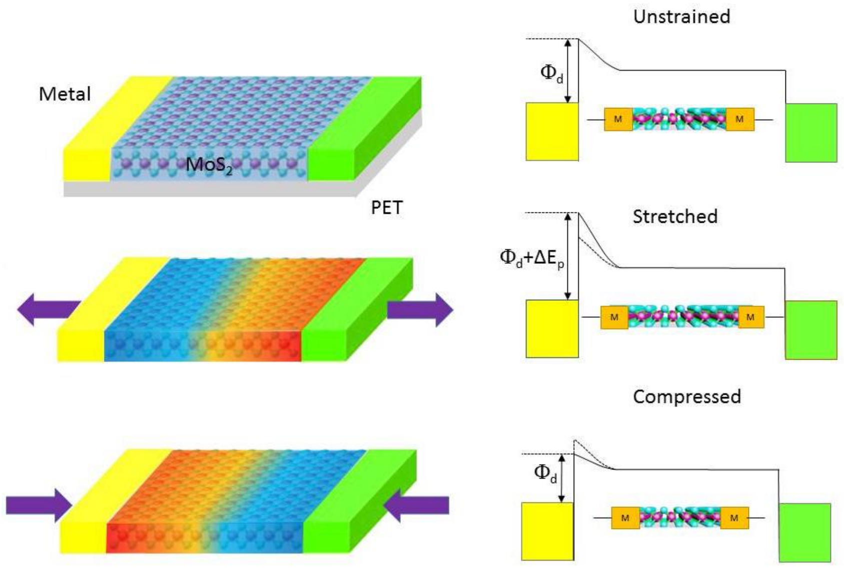
Abstract

Pieoztronic and piezo-phototronic are two emerging fields of flexible electronics and nanoelectronics using by piezoelectric semiconductor materials, such as ZnO, GaN, InN and CdS. Recent experiments shown piezoelectric and semiconductor properties of monolayer MoS_2, which have been applied as nanogenertor and piezotronic transistor. Two-dimensional piezoelectric semiconductor can be utilized for high-performance photovoltaic devices. In this paper, a two-dimensional material piezo-phototronic solar cell is studied theoretically based on a monolayer MoS_2 metal-semiconductor contact. The current-voltage characteristics, open circuit voltage, maximum output power, fill factor and power conversion efficiency have been studied for the piezo-phototronic solar cell. The modulation level of piezo-phototronic effect is presented to evaluate the performance under applied strain. The piezo-phototronic effect can increase the open circuit voltage 5.8% at strain of 1%. This principle can be a new way to develop high-performance two-dimensional solar cells.

Graphical Abstract



Monolayer MoS_2 shows piezoelectric and semiconductor properties in recent experiments, which have been used for nanogenertor and piezotronic transistor. Two-dimensional piezoelectric semiconductor can be applieded for piezo-phototronic solar cell. The modulation by piezo-phototronic effect can enhance the performance of monolayer MoS_2 solar cells.

Keywords

Piezotronic, Piezo-phototronic, solar cells; two-dimension material; MoS_2

1. Introduction

Piezoelectric semiconductor nanomaterials have been paid more and more attention over the past ten years, such as ZnO, GaN, InN and CdS. The new emerging fields of piezoelectronics and piezo-phototronics are established based on coupling of piezoelectric and semiconductor properties [1]. Since the invention of nanogenertors in 2006 [2-4], nanostructure piezoelectric semiconductors have been applied to multifunctional electromechanical devices, such as piezotronic field effect transistor [5], strain sensor [6], piezo-phototronic photocell [7], and LED [8]. Furthermore, integrated chips have been developed by nanowires array, such as taxel-addressable matrices [9] and photon-strain sensor arrays [10].

Recent experiments have revealed the coupling between piezoelectric and semiconductor properties in the single-atomic-layer MoS_2 [11], which promote the applications in powering nanodevices, energy harvesting and tunable electronics. Due to its excellent electronic, optical, catalytic and mechanical properties [12], monolayer MoS_2 can be fabricated as transistors [13, 14], photodetectors [15], and integrated circuits [16].

The principle of solar cell applies the built-in electric field to separate electron-hole pairs induced by incident photons in the p-n junction or metal-semiconductor contact. For piezo-phototronic solar cell (PSC), piezoelectric field can effectively assist the separation of photon-generated carriers [17, 18]. It should also be noted that piezo-phototronic effect can also improve the performance of two-dimensional material photodetector. High-performance, flexible and low-cost solar cell is research focus for large-area application, for example, building-integrated photovoltaic system [19]. Monolayer MoS_2 single junction device can be a good candidate for design of high-efficiency flexible solar cell, especially piezo-phototronic effect enhancing solar cell. There are several novel characteristics of monolayer MoS_2. First, incident sunlight can be absorbed up to 5% by monolayer MoS_2 within 1 nm, which is higher absorption about 10 times than GaAs and Si at same thickness [20]. Second, monolayer MoS_2 can be applied 11% in-plane strain [21]. Furthermore, monolayer MoS2 and other two-dimensional materials, such as WSe_2 and $MoSe_2$ can be fabricated as stacked multilayers solar cells [21]. This structure offers a low-cost way comparing with multi-junction high-efficiency solar cell.

In this manuscript, a two-dimensional material piezo-phototronic solar cell presents based on piezo-phototronics effect in monolayer MoS_2 materials [22, 23]. The schematic of the design is illustrated in Fig.1. The basic structure is a monolayer MoS_2 between two metal electrodes on the substrate. The left side of unstrained device is metal-semiconductor contact and right side is Ohmic contact, as shown in Fig. 1(a). For two-dimensional semiconductor materials, the metal-semiconductor-metal structure is commonly used in experiments. Because two back-to- back Schottky diode have opposite output voltage, the one side of 2D MSM device is used as solar cell and other side is electrode, that is to say, Ohmic contact. The device structure can also be p-n junction by using p-type and n-type 2D piezoelectric semiconductor materials. The piezoelectric polarization charges are induced at the contact of the piezo-phototronic solar cell under tensile and compressive strain. Piezoelectric field is able to increase or decrease the Schottky barrier at the contact as shown in Fig. 1(b) and Fig. 1(c), respectively. Piezoelectric field can enhance built-in potential, as well as assist to separate electron-hole pairs in metal-semiconductor contact. The parameters of piezo-phototronic solar cell are studied, such as current-voltage characteristics, open circuit voltage, maximum output power, fill factor, and power conversion efficiency. The scale ratio to evaluate the piezophototronic modulation on output characteristics has been studied for PSCs, and the open circuit voltage of monolayer MoS_2 PSC increases 5.8% with strain of 1%. This principle may provide a feasible design to fabricate high-efficiency and low-cost photovoltaic devices.

2. Piezo-phototronic modulation on two-dimensional materials solar cells

Semiconductor physics and piezoelectric theory are used to describe the properties of piezo-phototronic solar cell [17]. Piezoelectric charge induced by external applied strain can increase open circuit voltage of the solar cell, and thereby improve the performance. According to the piezo-phototronic theory, the total current density of 2D material solar cell is given by [17]:

$$J = J_{MS} \exp\left(\frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon_s kT}\right)\left[\exp\left(\frac{qV}{kT}\right) - 1\right] - J_{solar} \tag{1}$$

where J_{MS} is the saturation current density of metal-semiconductor, ρ_{piezo} is the density of the piezoelectric charges, W_{piezo} is the width of the charges distribution, k is the Boltzmann constant, the temperature T is 300K, ε_s is the relative dielectric constant, V is applied voltage and J_{solar} is the short circuit current density.

The density of the piezoelectric charges of 2D MoS_2 ρ_{piezo} can be obtained as [22]:

$$q\rho_{piezo} W_{piezo} = -e_{11} s_{11} \tag{2}$$

where e_{11} is piezoelectric constant, and s_{11} is applied strain.

The open circuit voltage is given by:

$$V_{oc} \approx \frac{kT}{q}\left\{\ln\left(\frac{J_{solar}}{J_{pn0}}\right) + \frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon_s kT}\right\} \tag{3}$$

The ratio γ can describe the modulation for open circuit voltage of piezo-phototronic solar cell by piezoelectric charges:

$$\gamma = \frac{\dfrac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon_s kT}}{\ln\left(\dfrac{J_{solar}}{J_{MS}}\right)} \tag{4}$$

This ratio γ can describe the piezo-phototronic modulation on output characteristics of piezo-phototronic solar cell.

Further, the output power can be obtained as:

$$P(V) = V \times J(V) = V \times \left(J_{MS} \exp\left(-\frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon_s kT} \right) \left[\exp\left(\frac{qV}{kT}\right) - 1 \right] - J_{solar} \right) \tag{5}$$

The voltage at the maximum output power V_m can be solved by the following equation:

$$V_m + \frac{kT}{q} \ln\left(\frac{qV_m}{kT} + 1 \right) = \frac{kT}{q} \left\{ \ln\left(\frac{J_{solar}}{J_{MS}} \right) + \frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon_s kT} \right\} \tag{6}$$

Thus, V_m changes with piezoelectric charges under applied strain. The current density at the maximum output power J_m and the maximum output power P_m can be calculated, respectively:

$$J_m = J_{MS} \exp\left(\frac{q^2 \rho_{piezo} W_{piezo}^2}{2\varepsilon_s kT} \right) \left[\exp\left(\frac{qV_m}{kT} \right) - 1 \right] - J_{solar} \tag{7}$$

$$P_m = V_m J_m \tag{8}$$

The fill factor, which is defined as the ratio of the maximum output power to the product of short circuit current and open circuit voltage, can be expressed as:

$$FF = \frac{P_m}{J_{solar} V_{oc}} = \frac{J_m V_m}{J_{solar} V_{oc}} \tag{9}$$

The power conversion efficiency (PCE) is extracted from the J-V curve. PCE is the general efficiency of the solar cell, which is defined as the ratio of generated electricity to incoming light energy:

$$PCE = \frac{J_{solar} V_{oc} FF}{P_{in}} \tag{10}$$

3. Results and discussion

The open circuit voltage, maximum output power, fill factor, and power conversion efficiency are calculated in the our calculation by using typical constants: The temperature is 300K, the relative dielectric constant of MoS_2 is 3.3 [16], the width of piezo-charges distribution W_{piezo} is 0.25 nm [17, 22], and the piezoelectric constant along a-axis for monolayer MoS_2 is 0.56 C/m^2 [24].

The model for calculations is shown in Fig.2 (a). A monolayer MoS_2 piezophototronic solar cell is based on the M-S contact at left side and Ohmic contact at right side. Fig.2 (b) presents the $J-V$ characteristics of the 2D PSC with applied strain varying from -1% to 1%, at a fixed short circuit current density as 3.15 mA/cm^2 [25]. The output power as a function of voltage at a fixed photocurrent density is shown in Fig.2 (c), indicating that current density increases with strain. The maximum power is obtained at V_m. Using by Eqn. (3) and Eqn. (8), the dependence of the open circuit voltage V_{oc} and maximum output power P_m on the applied strain are shown in the Fig.2 (d), respectively. The change of V_{oc} and P_m demonstrate the improvement on performance of 2D PSC by piezo-phototronic effect.

Fig.3 (a) shows the modulation ratio γ for piezo-phototronic solar cell changes with W_{piezo} while externally applied strain increases from -1% to 1%. While 2D material is stretched, the improvement on performance of 2D PSC will increase linearly. The width of piezo-charges distribution W_{piezo} is a key parameter of piezotronic and piezo-phototronic junction or contact. Fig.3 (b) shows γ as a function of strain when J_{solar} is 3.15 mA/cm^2 [25] and 22.36 mA/cm^2 [26]. The modulation ratio γ depends on the width of piezo-charge distribution W_{piezo}, as shown in Fig.3 (c). Due to piezo-phototronic effect, the modulation on output characteristics also is influenced by the width of piezo-charge distribution. The width of piezo-charge distribution is determined by not only different piezoelectric semiconductor, but also the metal materials of contact [27, 28]. The piezo-phototronic effect increases the open circuit voltage about 5.8% with strain of 1% while W_{piezo} is 0.25 nm. For W_{piezo} of 0.5 nm, the improvement on performance will reach up to 11.6% for this 2D PSC case. While strain of 2D material can be stretched to 11%, the ratio will reach even up to 10 times on the above case. This mechanism may provide a new way to develop high output performance two-dimensional solar cells.

Fig.3 (d) shows the ratio γ as a function of strain for different 2D materials: MoS_2, $MoSe_2$, and WSe_2. The piezoelectric constant is 0.56 C/m^2 (MoS_2), 0.48 C/m^2 ($MoSe_2$) and 0.27 C/m^2 (WSe_2) [24], respectively. Therefore, the modulation ratio γ can be considered as a scale factor for piezo-phototronic solar cell. It's obvious that the performance of piezo-phototronic solar cell can be tuned effectively by the applied strain in two-dimensional piezoelectric semiconductor materials. By solving the Eqn. (9) and Eqn. (10), two parameters to evaluate the performance of PSCs: FF and PCE are illustrated in Fig.4 (a) and Fig.4 (b), respectively, with the applied strain varying from -1.0% to 1.0%. The piezo-phototronic effect is able to improve fill factor and power conversion efficiency by increasing open circuit voltage, as a result, enhance the output performance of piezo-phototronic solar cell based on two-dimensional materials.

Piezoelectric properties have been discussed in other monolayer TMDs, such as $MoSe_2$ and WSe_2 [24]. The performance of piezoelectric solar cells fabricated by MoS_2, WSe_2[29] and $MoSe_2$[30] presents in Table.1. It shows that the modulation ratio of MoS_2 PSC is 2 and 4 times higher than $MoSe_2$ and WSe_2 PSCs. Table 2. presents the comparison between the recent experimental results based on piezoelectric semiconductor: MoS_2/InP [31] , MoS_2/GaAs [32] , MoS_2/Si and MoS_2/Graphene heterojunctions [25]. MoS_2/GaAs and MoS_2/InP have higher photocurrent density, which have the feasibility of applying piezo-phototronic effect to design the high performance ultra-thin solar cell.

4. Summary

In summary, we have presented the theoretical model of current-voltage characteristics of 2D piezoelectric solar cells. The open circuit voltage, maximum output power density, fill factor and power conversion efficiency are calculated for piezophototronic solar cells based on monolayer MoS_2. Piezophototronic solar cells have superior improvement on performance applied by piezophototronic effect, especially in open circuit voltage. Furthermore, monolayer MoS_2 shows potential for high performance piezophototronic solar cell comparing other two-dimensional materials. The theoretical results provide not only the physical picture for understanding the piezotronic and piezophototronic effect in two-dimensional solar cells but also the guidance for design of two-dimensional piezophototronic nanodevices.

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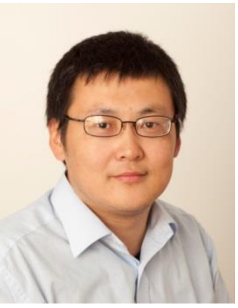
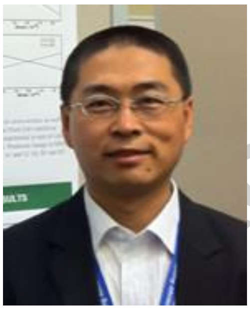
Jiaheng Nie received his B.E. in communication engineering from North China University of Water Resources and Electric Power in 2014. He is now pursuing his M.S. degree under the guidance of Professor Yan Zhang in School of Physical Electronics in UESTC. He is interested in the fields of piezotronics and piezo-phototronics



Lijie Li is an associate professor at Swansea University, UK. His research interests are design, modeling, fabrication, and characterization of MEMS, NEMS, sensors and actuators.



Yan Zhang is a professor at University of Electronic Science and Technology of China. He received his B. S. degree (1995) and Ph.D degree in Theoretical Physics (2004) from Lanzhou University. Then, he worked as associate Professor (2007) and Professor (2013) of Institute of Theoretical Physics in Lanzhou University. In 2009 he worked as research scientist in the group of Professor Zhong Lin Wang at Georgia Institute of Technology. His research interests include self-powered nano/micro system, piezotronic and modeling of nonlinear dynamics of NEMS.

Figure caption

Fig. 1. (a) Schematic and energy band diagram of a two dimensional piezophototronic solar cell fabricated using a monolayer MoS_2 metal-semiconductor contact at left side and Ohmic contact at right side. (b) Schematics and energy band diagram of the piezophototronic solar cell under compressive strain. (c) piezophototronic solar cells under tensile strain. The color code represents the distribution of the piezopotential at the two dimensional monolayer MoS_2.

Fig. 2. (a) Schematic of a monolayer MoS_2 piezophototronic solar cell based on the M-S contact (left side) and Ohmic contact (right side). (b) Relative current density as a function of voltage under various applied compressive strains (-0.9% to 0.9%). (c) Output power of a two-dimension MoS_2 piezophototronic solar cell as a function of voltage under various applied strains. (d) Open circuit voltage and maximum output power under various applied compressive strains.

Fig. 3. (a) The control ratio γ of piezophototronic solar cell changes with W_{piezo} and strain. (b) The control ratio γ of piezophototronic solar cell increases with strain from -1% to 1% while J_{solar} is 3.15 mA/cm^2 and 22.36 mA/cm^2. (c) The control ratio γ of piezophototronic solar cell as a function of W_{piezo} under applied strains of 0.2%, 0.6% and 1%. (d) The control ratio γ of piezophototronic solar cell as a function of strain with three kinds of 2D materials: MoS_2, $MoSe_2$, and WSe_2.

Fig. 4. (a) Fill factor and (b) Power conversion efficiency of piezophototronic solar cell based on monolayer MoS_2 under various applied strains from -1% to 1%.

Table:

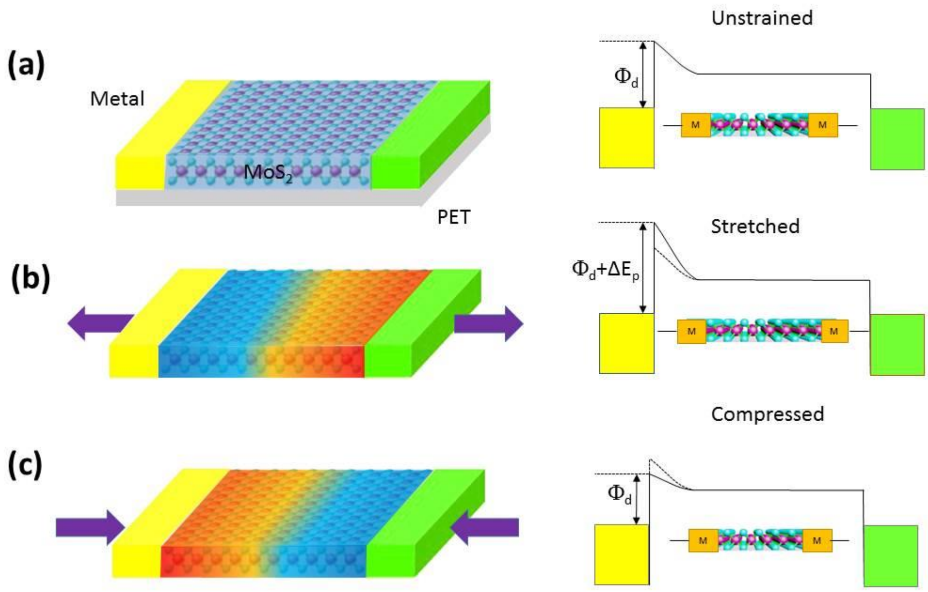
Table 1. Comparison between the Performance of Piezoelectric Solar cells Based on MoS_2, WSe_2 and $MoSe_2$.

Materials	V_{oc}^a(V)	J_{sc}^a(mA/cm^2)	P_m^a(mW/cm^2)	**FF**^{a}	V_{oc}^b**(V)**	P_m^b(mW/cm^2)	**FF**^{b}	**γ**
MoS_2	0.41	3.15	0.998	77.30%	0.434	10.69	82.74%	0.058
WSe_2	0.82	17.39	12.29	86.19%	0.831	12.49	87.56%	0.014
$MoSe_2$	0.62	6.05	3.12	83.04%	0.640	3.23	86.21%	0.033

(a. These parameters are calculated without applied strain and b. with applied strain of 1%).

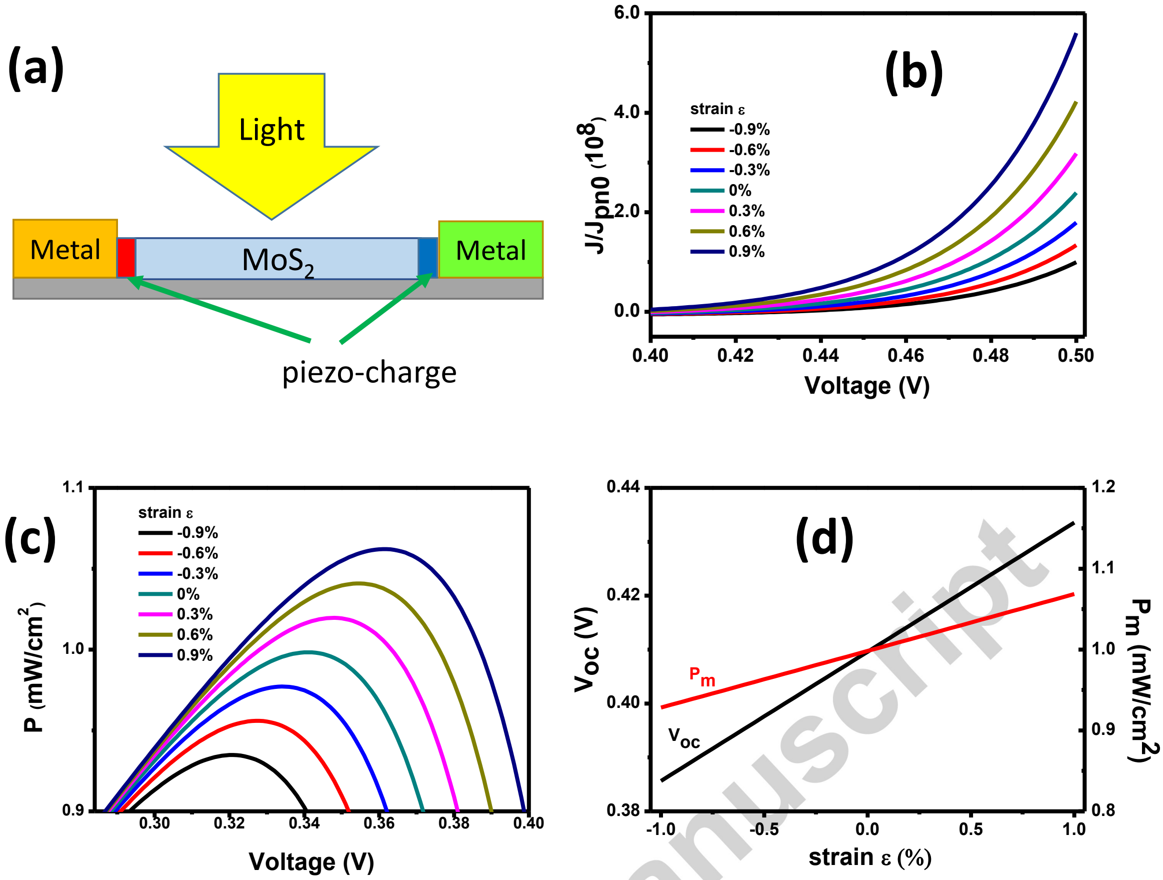
Table 2. Comparison between the Performance of Piezoelectric Solar Cells Based on MoS_2/InP , MoS_2/GaAs, MoS_2/Si , MoS_2/Graphene and $MoSe_2$/GaN.

Materials	V_{oc}(V)	J_{sc}(mA/cm^2)	P_m(mW/cm^2)	**FF**
MoS_2/InP	0.39	21.8	6.51	76.51%
MoS_2/GaAs	0.55	20.87	9.36	81.52%
MoS_2/Si	0.41	22.36	7.09	77.30%
MoS_2/Graphene	0.33	3.15	0.766	73.73%
$MoSe_2$/GaN	0.62	6.05	3.12	83.04%



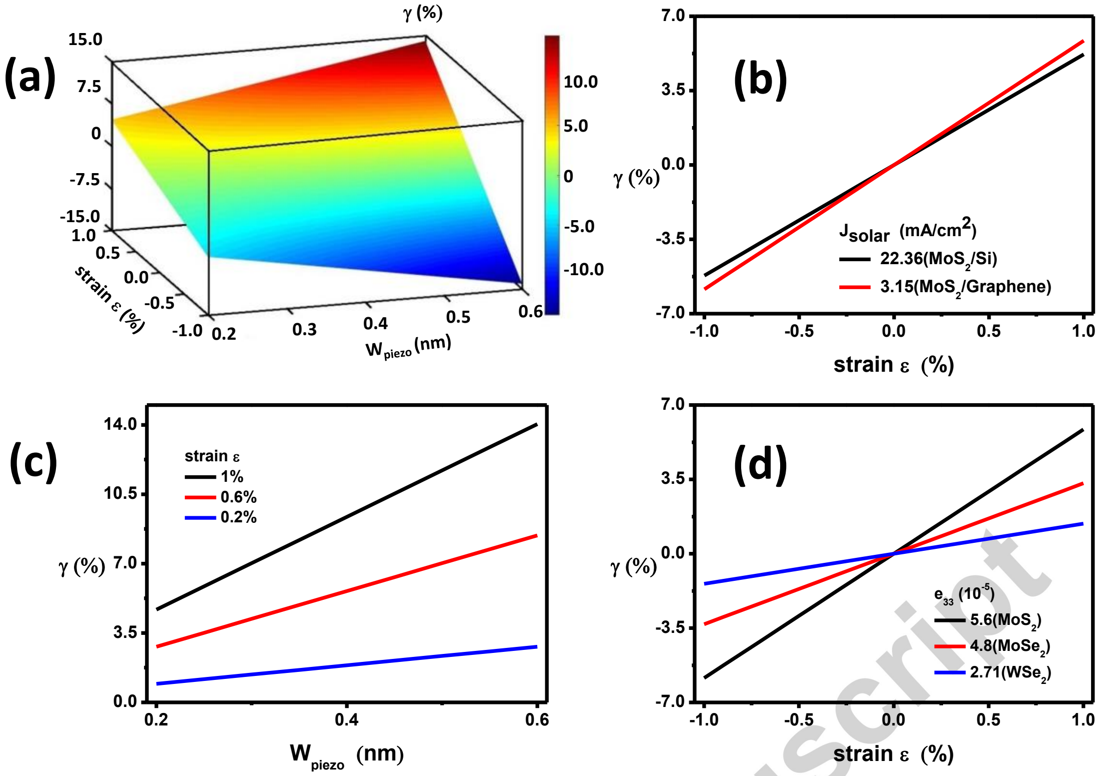
(a)
Metal
MoS2
PET
(b)
(c)
Unstrained
Φd
M
M
Stretched
Φd+ΔEp
Compressed

Fig. 1



(a)
Light
Metal
MoS2
Metal
piezo-charge
(b)
strain ε
-0.9%
-0.6%
-0.3%
0%
0.3%
0.6%
0.9%
J/Jpn0 (10^8)
Voltage (V)
(c)
strain ε
-0.9%
-0.6%
-0.3%
0%
0.3%
0.6%
0.9%
P (mW/cm2)
Voltage (V)
(d)
Pm
Voc
Voc (V)
Pm (mW/cm2)
strain ε (%)

Fig. 2



(a)
γ (%)
15.0
7.5
0
-7.5
-15.0
10.0
5.0
0
-5.0
-10.0
1.0
0.5
0.0
-0.5
-1.0
strain ε (%)
0.2
0.3
0.4
0.5
0.6
W piezo (nm)
(b)
7.0
3.5
0.0
-3.5
-7.0
γ (%)
J solar (mA/cm2)
22.36(MoS2/Si)
3.15(MoS2/Graphene)
-1.0
-0.5
0.0
0.5
1.0
strain ε (%)
(c)
14.0
10.5
7.0
3.5
0.0
γ (%)
strain ε
1%
0.6%
0.2%
0.2
0.4
0.6
W piezo (nm)
(d)
7.0
3.5
0.0
-3.5
-7.0
γ (%)
e33 (10-5)
5.6(MoS2)
4.8(MoSe2)
2.71(WSe2)
-1.0
-0.5
0.0
0.5
1.0
strain ε (%)

Fig. 3

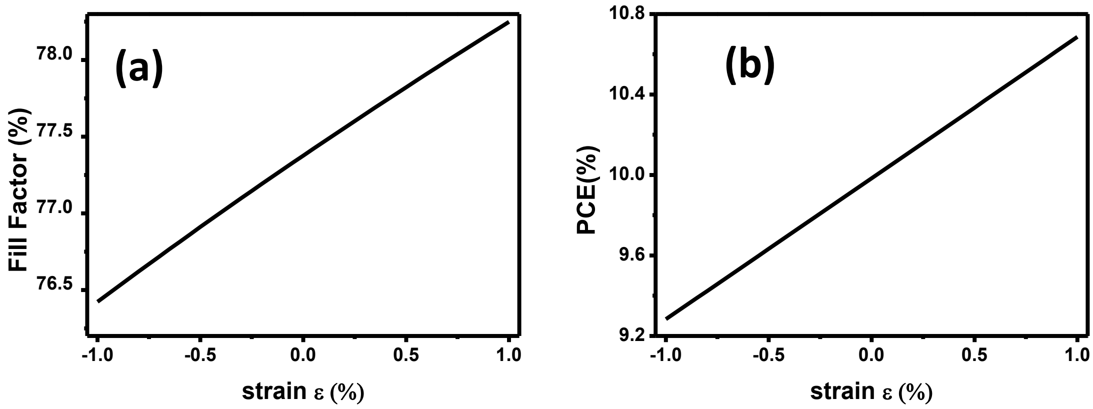


Fig. 4

Highlights

- Two-dimension piezo-phototronic solar cells can be a promising high-performance photovoltaic device, which have tunable properties under external applied strain.
- The piezo-phototronic effect can increase the open circuit voltage 5.8% at strain of 1%.
- The theoretical model provides a feasible structure of two dimensional piezo-phototronic solar cells for improvement of performance.