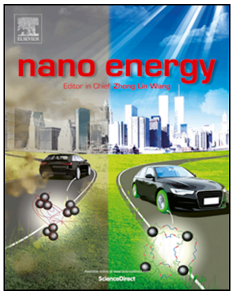

High-performance piezo-phototronic multijunction solar cells based on single-type two-dimensional materials

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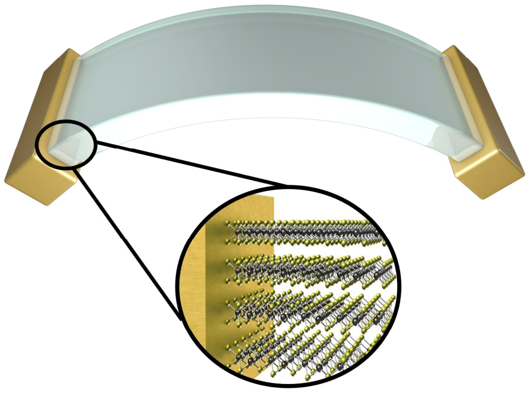
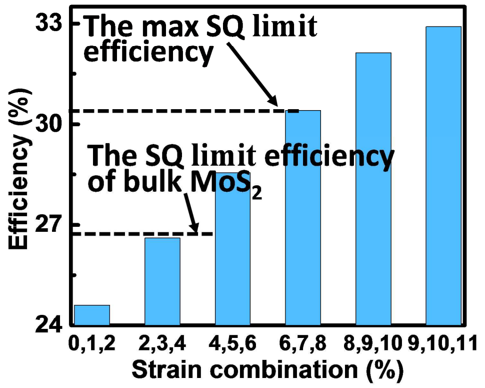
Credit Author Statement

Gyan Michael: Conceptualization, Methodology, Formal analysis, Writing- Original draft preparation, Validation; **Yaming Zhang:** Conceptualization, Methodology, Formal analysis, Writing- Original draft preparation, Validation; **Jiaheng Nie:** Sketch, Formal analysis, Validation; **Dongqi Zheng:** Methodology, Formal analysis; **Gongwei Hu:** Formal analysis, Validation; **Ruhao Liu:** Formal analysis, Validation; **Minjiang Dan:** Formal analysis, Validation; **Lijie Li:** Writing- Reviewing and Editing; **Yan Zhang:** Supervision, Conceptualization, Methodology, Formal analysis, Writing- Reviewing and Editing

Graphical Abstract





The externally applied strain can modulate material bandgap and generate piezoelectric charges. The piezo-phototronic multijunction solar cell consisted only of single type two-dimensional material is proposed by utilizing bandgap engineer and piezo-phototronic effect. The efficiency of piezo-phototronic multijunction solar cell can theoretically reach over 33% and it has theoretically exceeded Schckley-Queisser limit. This offer a guidance to design ultrahigh performance piezo-phototronic photovoltaic device.

High-performance Piezo-phototronic Multijunction Solar Cells based on Single-type Two-dimensional Materials

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Abstract

Piezotronics and piezo-phototronics based on the third-generation semiconductor (such as ZnO, GaN, CdS, and monolayer chalcogenides) and two-dimensional materials, have attracted increasing attention due to the coupling characteristic of piezoelectric, photon excitation, and semiconductor properties. Strain can not only induce piezoelectric charges but also modulate bandgap of piezotronic materials. In this paper, we propose a structure of piezo-phototronic multijunction solar cell based on single-type two-dimensional piezoelectric semiconductor materials. By using the theory of detailed balance limit, the open circuit voltage and short circuit current of this piezo-phototronic multijunction solar cell are calculated. The results indicate that power conversion efficiency of the piezo-phototronic multijunction solar cell can theoretically reach to 33%, under the blackbody of temperature 6000K, which is higher than the well-known theoretical Shockley-Queisser limit. This work provides guidance to design the next generation ultra-high performance piezo-phototronic solar cells.

Keywords: piezo-phototronics, bandgap, two-dimensional materials, multi-junction solar cells, detailed balance limit

1. Introduction

Owing to coupling of piezoelectric and semiconductor characteristic, the third-generation semiconductor materials, such as ZnO, CdS, GaN, InN, and monolayer chalcogenides have attracted increasing research interests [1-3]. Strain induced piezoelectric charges control carrier transport, generation, separation, and recombination to design novel high performance piezotronic and piezo-phototronic devices [4]. Inspired by the requirement of high performance and low power consumption, a series of piezotronic and piezo-phototronic devices have been designed, such as nanogenerator [5-7], flexible stain sensors [8], piezotronic field-effect transistors [9], piezo-phototronic solar cell [10], piezo-phototronic photodetectors [11], and LEDs [12]. Piezo-phototronic effect can tune the luminescence based on monolayer MoS_2 and ZnO nanowires for designing highly sensitive optoelectronic devices [13-15]. Additionally, piezoelectric field of the interface can trigger the topological phase transition from normal insulator to topological insulator state to realize piezotronic devices with ultrahigh ON/OFF radio due to piezotronic effect [16, 17]. Non-uniform strain can be used to improve the performance of piezotronic devices by enhancing piezoelectric polarization [18]. The piezotronics offers a novel way to develop high performance devices for energy, artificial intelligence and human-integrated technologies [2].

Multijunction solar cell as the next generation photovoltaic device, has demonstrated rather high theoretical and experimental efficiency and it is expected to surpass Shockley-Queisser limit [19-21]. Connecting two or more solar cells can effectively reduce the lattice thermalization losses to realize more power conversion efficiency [19]. Traditional multijunction solar cell are constructed by parallel/tandem solar sub-cells based on different band gaps, which use several types of semiconductor materials [22, 23]. There exists engineering and manufacturing complexity for traditional multijunction solar cell. Monolayer two-dimensional (2D) materials, especially transition metal dichalcogenides including MoS_2, $MoSe_2$, WS_2, WSe_2, etc. have several novel characteristics for photo-detection [24], photoluminescence [25], and photovoltaic devices [26].

Strain can change bandgap of two dimensional material [27], and the stretching limit of such materials can reach to 11% in the form of in-plane strain [28]. In additional, strain induced piezoelectric charges can effectively decrease Schottky Barrier of metal-semiconductor to diminish thermalization voltage loss, and the performance of solar cell can be enhanced [29]. Therefore, the piezo-phototronic multijunction solar cell based on single-type 2D materials can be realized by applying different strains to sub-cells based on the same 2D material and it has promising applications attributed to high conversion efficiency and simple engineered technical requirements.

In this paper, the structure of piezo-phototronic multi-junction solar cells based on a single type two-dimensional material is proposed. Figure 1(a) illustrates the structure of this parallel piezo-phototronic multijunction photovoltaic device. MoS_2 stacking layers as the light absorbing materials are sandwiched between two contacts. The left side is Schottky contact, which can separate the photon-generated carriers by the Schottky barrier. The other side is simplified as an ohmic contact for the transportation of current without rectification. Modulation on bandgap and piezo-charges (inset) with different strains are depicted in Fig.1(b). The applied strain not only influences the bandgap of two-dimensional semiconductors but also generates piezoelectric charges. The bandgap of monolayer MoS_2 varying with externally applied strain, and the bandgap obviously decrease from 1.82eV to 1.17eV. This means MoS_2 can absorb photons of the lower energy with increasing strain. Moreover, the piezoelectric charges increase obviously with strain, and it can exceed piezoelectric charges of traditionally piezoelectric semiconductor since monolayer MoS_2 can withstand up to 11% strain. Meanwhile, the sun is assumed to be a blackbody at temperature 6000K. Figure 1(c) demonstrate the power density for a blackbody emitter at temperature T_s=6000K. Additionally, the photon energy above solar cell material bandgap can be absorbed and generate photocurrent. According to Shockley-Queisser theory, Figure 1(d) illustrate the overall solar cell efficiency as a relation about semiconductor bandgap for single junction solar cell. The efficiency can have a maximum value at 1.3 eV and reach about 31%. In the theory of electronic circuit, piezo-phototronic multijunction solar cell is equivalent to a battery comprised of several sub-cells connected in parallel. Sub-cells demand matching open-circuit voltage (V_{oc}) to reduce intrinsic loss. In this paper, piezo-phototronic effect can both decrease the mismatch of V_{oc} from sub-cells of different layers and enhance the performance of piezo-phototronic multijunction solar cell. As a result, the power conversion efficiency can reach about 33% for a triple junction piezo-phototronic multijunction solar cell consisting of 15 stacked monolayer MoS_2 when we assume the sun as a blackbody of temperature 6000K. Significantly, the efficiency can surpass the Shockley-Queisser limit. Therefore, the piezo-phototronic multi-junction solar cells based on single type two-dimensional material is hoped to surpass the well-known theoretical Shockley-Queisser limit, and it can be realized by utilizing photo-phototronic effect and deformation potential.

2. Basic theory of piezo-phototronic multijunction solar cell

2.1 Theoretical analysis of 2D multijunction solar cell

2.1.1 Theory of detailed balance limit

In photovoltaic basic theory, the solar cell can absorb part of incident solar flux, and convert this energy to electric power. The absorption can cause generation of electron-hole pairs, which can be extracted and recombined by an external circuit. This process can drive electrons to flow in the external circuit. To simplify, we assume following conditions for calculating detail balance model: (1) all photons with energy lower than the material bandgap are transmitted; (2) per absorbed photon generates one electron hole pair (quantum efficiency QE=1); (3) only radiative recombination exists; (4) all emitted thermal photons can be reflected back to the solar cell; (5) reflective and resistive losses are neglected.

In previous studies [30-32], the conversion efficiency of solar cell is calculated by utilizing Shockley-Queisser theory. The previous results qualitatively consistent under a blackbody with temperature 6000K and AM1.5 standard, which have minor numerical differences because spectral power density have minor differences. Therefore, the results of SQ limitation is same under AM1.5 standard. We assume the sun as a blackbody with temperature T_s=6000K, similar to previous investigation. According to Planck's law, the spectral photon flux is given [30, 31]

$$F_s = f_\omega \frac{2\pi}{h^3c^2}\frac{E^2}{e^{E/kT_s}-1} \tag{1}$$

Where the h and c are Planck's constant and speed of light, respectively. k is Boltzmann's constant, and E represent energy of photons, f_ω is geometry factor and $f_\omega = 2.18\times10^{-5}$ [30]. For a solar cell, the current density generated by absorbing the incident photons is

$$J_{sc} = q\int_0^\infty a(E)F_s dE = qf_\omega\int_0^\infty a(E)\frac{2\pi}{h^3c^2}\frac{E^2}{e^{E/kT_s}-1}dE \tag{2}$$

In this equation, $a(E)$ is absorption ratio which represents probability of absorbing photons of energy E, and q is charge of an electron. When this solar cell is not illuminated, it absorbs and emits similar to a blackbody at ambient temperature T_c=300K since the solar cell is thermodynamic equilibrium with its surroundings ambient temperature. The solar cell is not in thermal equilibrium with its surroundings while the cell is in illumination. According to previous study [31], the reverse saturation current J_0 is given by

$$J_0 = f_g \frac{2\pi q}{h^3c^2}\int_0^\infty e(E)E^2e^{-E/kT_c}dE \tag{3}$$

where the $e(E)$ is the emissivity which is probability of emitting photons of energy E and $e(E)=a(E)$ because the current density is balanced, the f_g is a geometry factor and f_g=2 [33] since emission occurs at both the front and back surfaces. At open circuit condition, the current density is zero and the open circuit voltage V_{oc} can be obtained by [29]

$$V_{oc} = \frac{kT_c}{q}[\ln(\frac{J_{sc}}{J_0})+1] \tag{4}$$

In this study, we assume $a(E)$=0 for photons of energy $E<E_g$. Moreover, the absorption of light can reach 20% in the photon energy range above bandgap for monolayer MoS_2. Therefore, we can assume $a(E)$=50% for per part consisting of five monolayer MoS_2 in the photon energy range above bandgap.

2.1.2 Theoretical analysis of multijunction solar cell based on detailed balance limit

For a parallel triple junction solar cell, the structure is similar to Figure 2 (a).The bandgaps of Part 1, Part 2 and Part 3 are respectively E_g^1, E_g^2 and E_g^3, where $E_g^1 > E_g^2 > E_g^3$. According to equation (1), the short circuit current density of sub-cells is given by

$$\begin{aligned} J_{sc}^1 &= qf_\omega \int_{E_g^1}^{\infty} a(E)\frac{2\pi}{h^3c^2}\frac{E^2}{e^{E/kT_s}-1}dE \\ J_{sc}^2 &= qf_\omega \int_{E_g^2}^{\infty} a(E)\frac{2\pi}{h^3c^2}\frac{E^2}{e^{E/kT_s}-1}dE - a(E)J_{sc}^1 \\ J_{sc}^3 &= qf_\omega \int_{E_g^3}^{\infty} a(E)\frac{2\pi}{h^3c^2}\frac{E^2}{e^{E/kT_s}-1}dE - a(E)J_{sc}^2 - a(E)J_{sc}^1 \end{aligned} \tag{5}$$

where J_{sc}^1 J_{sc}^2 and J_{sc}^3 are current density of sub-cells (Part 1, Part 2 and Part 3), respectively. According to Kirchhoff's law, the total current density of multijunction solar cell is sum of current density of all sub-cells. Current density-Voltage (J-V) properties of the parallel solar cell are calculated by

$$\begin{aligned} J(V) &= \sum_{i=1}^{2,3}\left(J_0^i[\exp(\frac{qV}{kT_c})-1] - J_{sc}^i \right) \\ J_{sc}^p &= J(V=0), \quad J(V_{oc}^0)=0 \end{aligned} \tag{6}$$

In the equation, Subscript *i* is the number of one sub-cell in the parallel solar cell. J_0^i and J_{sc}^i are saturation current density and short circuit density of per sub-cell, respectively. J_{sc}^p and V_{oc}^0 are total short circuit current density and open circuit voltage, respectively.

2.2 Analytical model of 2D piezo-phototronic multijunction solar cell

In our study, we adopt stacked multi-monolayer MoS_2 as material of solar cell. While the strain is applied at piezoelectric semiconductor materials, the piezoelectric charges are generated on both side of materials and the bandgap can be varied. For this work, we assume the applied strains of Part 1, Part 2, and Part 3 are denoted as s_{11}^1, s_{11}^2 and s_{11}^3 respectively. The bandgap of each sub-cell is calculated by using

$$\begin{aligned} E_g^1 &= E_g^0 - 100\times E_s s_{11}^1 \\ E_g^2 &= E_g^0 - 100\times E_s s_{11}^2 \\ E_g^3 &= E_g^0 - 100\times E_s s_{11}^3 \end{aligned} \tag{7}$$

where E_g^0 is the material bandgap without strain, E_s is variation of bandgap while 1% strain is applied by the material. Additionally, the piezoelectric charges can vary the Schottky barrier, and it is given by [34]

$$\Delta\phi = \frac{q e_{11} s_{11} W_{piezo}}{2\varepsilon} \tag{8}$$

where e_{11} and W_{piezo} are piezoelectric constant and piezoelectric charge distribution width, s_{11} and ε are applied strain and material dielectric constant, $\Delta\phi$ is Schottky Barrier Height variation caused by strain induced piezoelectric charges. Considering equations (5), (7), the current density of sub-cell is

$$\begin{aligned} J_{sc}^{1} &= q f_{\omega} \int_{E_g^0 - E_s s_{11}^1}^{\infty} a(E) \frac{2\pi}{h^3 c^2} \frac{E^2}{e^{E/kT_s} - 1} dE \\ J_{sc}^{2} &= q f_{\omega} \int_{E_g^0 - E_s s_{11}^2}^{\infty} a(E) \frac{2\pi}{h^3 c^2} \frac{E^2}{e^{E/kT_s} - 1} dE - a(E) J_{sc}^{1} \\ J_{sc}^{3} &= q f_{\omega} \int_{E_g^0 - E_s s_{11}^3}^{\infty} a(E) \frac{2\pi}{h^3 c^2} \frac{E^2}{e^{E/kT_s} - 1} dE - a(E) J_{sc}^{2} - a(E) J_{sc}^{1} \end{aligned} \tag{9}$$

Through equations (6), (8), and (9), the electric characteristic of the piezo-phototronic multijunction solar cell is

$$\begin{aligned} J(V) &= \sum_{i=1}^{2,3} \left(J_0^i \exp(-\frac{q e_{11} s_{11}^i W_{piezo}}{2\varepsilon k T_c})[\exp(\frac{qV}{kT_c}) - 1] - J_{sc}^i \right) \\ J_{sc}^{p} &= J(V=0), \quad V_{oc} = V_{oc}^0 + \frac{P_z W_{piezo}}{2\varepsilon} \end{aligned} \tag{10}$$

where V_{oc}^0 is open circuit voltage without piezoelectric charges, V_{oc} is open circuit voltage of MJSC induced by piezoelectric charges, and P_z is piezoelectric charges and $P_z = e_{11} s_{11}$.

3. Results and Discussion

In this investigation, we adopt typical constants as following: the piezoelectric constant of monolayer MoS_2 is 0.56C/m^2 [35, 36]. Previous works show monolayer MoS_2 can apply strain up to 11% strain before fracture [28] . Moreover, these works [37, 38] have demonstrated monolayer MoS_2 and few layer MoS_2 will experience elastic deformation until maximum strain of MoS_2. Piezoelectric constant of various piezoelectric materials is steadily at different strain [39] . Thus, the piezoelectric constant of five monolayer MoS_2 is assumed a constant. In addition, the piezoelectric constant of five monolayer MoS_2 is assumed that is equal to monolayer due to each monolayer of five-layer MoS_2 stacked along the same polarized direction [40]. Therefore, the piezoelectric constant of five monolayer MoS_2 is 0.56C/m^2. the relative dielectric constant is 3.3 [41], the piezoelectric charges distribution width W_{piezo} is 0.25nm [34], the material bandgap is 1.82eV [42], and E_s is 59meV [42].

Figure 2(a) demonstrates the structure of piezotronic multijunction solar cell, and it consists of three sub-cells (top cell: Part 1, middle cell: Part 2, bottom cell: Part 3). Each sub-cell contains five stacked monolayer MoS_2. Top, middle and bottom cells are applied different strains, respectively. As shown in

Figure 2(b), the short circuit current density (J_{sc}) is as a function of different strain combinations. While the applied strain combination increases, the bandgap can decrease, and more photons are absorbed. Therefore, the J_{sc} increases. Figure 2(c) show that the open circuit voltage (V_{oc}) will decrease with enhancing applied strain combination. V_{oc} is dependent on the material bandgap and V_{oc} is slightly lower than the bandgap owing to voltage loss, strain can decrease V_{oc} through reducing material bandgap. Moreover, MoS_2 is piezoelectric semiconductor, and strain induced piezoelectric charges can decrease voltage loss. Figure 2(d) shows the maximum power density of the piezo-phototronic multijunction solar cell at different strain combinations. Since strain increases photon absorption and strain induced piezoelectric charges decrease voltage loss, the maximum power density increases with the enhanced applied strain combination.

Figures 3 (a) and (b) show respectively short circuit current density and open circuit voltage with relation about strains of top and middle cell while the strain of bottom cell is fixed at 11%. It is clear that short circuit current density can increase with enhancing strains of top and middle cell at a fixed strain of bottom cell (11%). At the same time, the open circuit voltage decreases as a whole. Figures 3 (c) and (d) illustrate severally short circuit current density and open circuit voltage as functions of strains of middle and bottom cell while no strain is applied at top cell. Similar to above, the short circuit current density can increase and the open circuit voltage decrease with increasing strain of middle and bottom cell at a top cell being zero strain. This is because the strain changes the band gap, more photons are absorbed, hence short circuit current density increases. However, bandgap also limits open circuit voltage of solar cell, therefore open circuit voltage decreases as a whole. As shown in Figure 3 (b), open circuit also shows locally abnormal phenomenon with increasing strains of top and middle cell. This is due to voltage matching of different sub-cells in the parallel multijunction solar cell.

Figure 4(a) demonstrates the fill factor (FF) of piezo-phototronic multijunction solar cell at different strain combinations. It is clearly shown that the FF can decrease with increasing the applied strain combination, consistent with theory of single junction solar cell. Additionally, Figure 4(b) illustrate the efficiency of piezo-phototronic multijunction solar cell at different strains combination. The efficiency of piezo-phototronic multijunction solar cell increases while the applied strains combination is increased. Significantly, the efficiency can exceed the Shockley-Queisser limit efficiency of 1.82eV (bandgap of MoS_2) while the strains combination of three sub-cells achieve 2%, 3%, 4%. Moreover, the efficiency of piezo-phototronic multijunction solar cell can achieve over the maximum Shockley-Queisser limit efficiency (which is at 1.3 eV) while the strains combination of three sub-cells exceed 6%, 7%, 8%. Figure 4(c) illustrates that the power conversion efficiency is enhanced with increasing strain of top and middle cell while the strain of bottom cell is fixed at 11%, and the maximum efficiency value can surpass 33%. Moreover, Figure 4(d) shows that the power conversion efficiency can increase with increasing applied strains of middle and bottom cell at top cell being at zero strain. This is a result affected by deformation potential and piezo-phototronic effect.

The conversion efficiency of semiconductors can be enhanced by piezo-phototronic effect. The conversion efficiency of ZnO and GaN are calculated by utilizing this model, the material parameters using for calculation is listed in Supplementary Table 1, and the result is shown in Supplementary Figure 1. The calculations show that strain can effectively enhance conversion efficiency of piezo-phototronic multijunction solar cell based on thin semiconductor (ZnO and GaN). This is consistent with the result in Figure 4. As shown in Supplementary figure 1, efficiency of piezo-phototronic multijunction solar cell based on GaN is increased from 6.12% to 14%, and it has surpassed the Shockley-Queisser limit (7%). For ZnO, efficiency of piezo-phototronic multijunction solar cell is enhanced from 6.12% to 6.43%. According to experimental measurement [43], the maximum strain of ZnO nanowire is typical 2.5%. ZnO has strain limitation to break the Shockley-Queisser limit of ZnO (7%). Significantly, this phenomenon that strain can change material bandgap universally exit in semiconductor material. For junction of non-piezoelectric semiconductor and piezoelectric semiconductor, strain induced piezoelectric charges at the interface can also adjust open circuit voltage of solar cell [3]. Therefore, the principle can also be used for junction of non-piezoelectric and piezoelectric semiconductor to enhance conversion efficiency. Two-dimensional materials have better stretching properties and withstand higher strain than thin piezoelectric semiconductor (ZnO, GaN, InN, and CdS etc). The conversion efficiency of piezo-phototronic multijunction solar cell based on MoS2 can be significant increased and it surpass the maximum Shockley-Queisser limit (31%). Thus, two-dimensional semiconductor materials are good candidate to high performance piezo-phototronic solar cell.

In this works, strain can obviously vary bandgap of material, and MoS_2 at different strains can be used as sub-cells of piezo-phototronic solar cell to absorb photons of different energy. Significantly, the open circuit voltage will decrease while bandgap decrease. However, the drop of open circuit voltage is minished owing to strain induced piezoelectric potential [29, 36]. This enhance voltage match of parallel piezo-phototronic multijunction solar cell. This is unique advantages of piezoelectric semiconductor. At same time, previous work [44] show two-dimensional materials is produced to be 100m long rolls, such excellent performance will be of great value in engineering production of roll to roll. Moreover, conversion efficiency of series multijunction solar cell has been investigated [19, 22]. Since series structure generally exit trouble of current match, this greatly limits the combination range of the optional material band gaps. In this investigation, we adopt parallel piezo-phototronic multijunction solar cell. Strain induced piezoelectric potential can improve voltage match which generally exist in parallel structure [29], so the piezo-phototronic multijunction solar cell have less limit in optional materials, and this also have less difficulty in Engineering design. This study demonstrates a method to break Shockley-

Queisser limit by utilizing piezo-phototronic effect and deformation potential to realize multijunction solar cell only consisting of homogenous material.

4. Conclusion

In summary, we firstly propose a structure of the piezo-phototronic multijunction solar cell based on single type 2D materials and investigate its electric characteristics and power conversion efficiency. For this piezo-phototronic devices, the short circuit current density and open circuit voltage can be modulated by the applied strain since strain can tune bandgap and generate piezoelectric charges. Furthermore, the power conversion efficiency can reach about 33% for this triple-junction piezo-phototronic multijunction solar cell while we assume the sun as a blackbody of temperature 6000K. It has exceeded Shockley-Queisser limit of bulk MoS_2 with strains combination (2%, 3%, 4%), and the maximum Shockley–Queisser limit (30.5% of bandgap 1.3eV) with strains combination (6%, 7%, 8%). Therefore, the piezo-phototronic multijunction solar cell based on single type 2D materials have promising potential application. The work paves the way to realizing high performance solar cells with the strain induced piezo-phototronic effect.

Figure caption

Figure 1 (a) Schematic of two-dimensional piezo-phototronic multijunction solar cells; (b) Direct band gap, Piezo-charge (inset), as a function of strain; (c) Spectral power density blackbody at temperature T_s=6000K) illustrates above-bandgap absorption from a solar cell; (d) the detailed balance limit of efficiency.

Figure 2 (a) The parallel structure of piezo-phototronic multijunction solar cell; (b) Open circuit voltage (V_{oc}), (c) Short circuit current density (J_{sc}), (d) Maximum power density (P_m) on different combinations of strains of three parts of the parallel piezo-phototronic multijunction solar cell;

Figure 3 (a) Short circuit current density, (b) Open circuit voltage as a function about strains of top and middle cell while strain of bottom cell is fixed at 11%; (c) Short circuit current density (d) Open circuit voltage as a relation about strain of middle and bottom strain while no strain is applied at top cell.

Figure 4 (a) Fill factor, (b) Efficiency on different combinations of strains of three parts of parallel piezo-phototronic multijunction solar cell; Efficiency as a function of (c) strains of top and middle cell while strain of top cell is fixed at 11%; (d) strains of middle and bottom cell while no strain is applied at top cell.

Reference

[1].Wu W and Wang Z L Piezotronics and piezo-phototronics for adaptive electronics and optoelectronics. Nature Reviews Materials, 2016, 1.

[2].Wang Z L, Wu W, and Falconi C Piezotronics and piezo-phototronics with third-generation semiconductors. MRS Bulletin, 2018, 43: 922-927.

[3].Pan C, Zhai J, and Wang Z L Piezotronics and Piezo-phototronics of Third Generation Semiconductor Nanowires. Chem Rev, 2019, 119: 9303-9359.

[4].Zhang Y, Leng Y, Willatzen M, et al. Theory of piezotronics and piezo-phototronics. MRS Bulletin, 2018, 43: 928-935.

[5].Wang Z L and Song J Piezoelectric nanogenerators based on zinc oxide nanowire arrays. Science, 2006, 312: 242-6.

[6].Wang X, Song J, Liu J, et al. Direct-current nanogenerator driven by ultrasonic waves. Science, 2007, 316: 102-5.

[7].Qin Y, Wang X, and L. W Z Microfibre-nanowire hybrid structure for energy scavenging. Nature, 2008, 451: 809-13.

[8].Zhou. J, Gu. Y, Fei. P, et al. Flexible Piezotronic Strain Sensor. Nano Lett., , 2008, 8: 3035-3040.

[9].Wang X, Zhou J, Song J, et al. Piezoelectric Field Effect Transistor and Nanoforce Sensor Based on a Single ZnO Nanowire. 2006, 6: 2768-2772.

[10].Hu Y, Zhang Y, Chang Y, et al. Optimizing the Power Output ofa ZnO Photocell by Piezopotential. 2010: 4220–4224.

[11].Yang Q, Guo X, Wang W, et al. Enhancing sensitivity of a single ZnO micro-/nanowire photodetector by piezo-phototronic effect. Acs Nano, 2010, 4: 6285-6291.

[12].Yang Q, Wang W, Xu S, et al. Enhancing light emission of ZnO microwire-based diodes by piezo-phototronic effect. Nano Lett, 2011, 11: 4012-7.

[13].Zhang Y and Li L Piezophototronic effect enhanced luminescence of zinc oxide nanowires. Nano Energy, 2016, 22: 533-538.

[14].Li L and Zhang Y Controlling the luminescence of monolayer MoS2 based on the piezoelectric effect. Nano Research, 2017, 10: 2527-2534.

[15].Zhang Y, Nie J, and Li L Piezotronic effect on the luminescence of quantum dots for micro/nano-newton force measurement. Nano Research, 2018, 11: 1977-1986.

[16].Hu G, Zhang Y, Li L, et al. Piezotronic Transistor Based on Topological Insulators. ACS Nano, 2018, 12: 779-785.

[17].Dan M, Hu G, Li L, et al. High performance piezotronic logic nanodevices based on GaN/InN/GaN topological insulator. Nano Energy, 2018, 50: 544-551.

[18].Zhang Y, Hu G, Zhang Y, et al. High performance piezotronic devices based on non-uniform strain. Nano Energy, 2019, 60: 649-655.

[19].Henry C H Limiting efficiencies of ideal single and multiple energy gap terrestrial solar cells. Journal of applied physics, 1980, 51: 4494-4500.

[20].Brown A S and Green M A Detailed balance limit for the series constrained two terminal tandem solar cell. Physica E: Low-dimensional Systems and Nanostructures, 2002, 14: 96-100.

[21].Connolly J P, Mencaraglia D, Renard C, et al. Designing III–V multijunction solar cells on silicon. Progress in Photovoltaics: Research and Applications, 2014, 22: 810-820.

[22].Abdul Hadi S, Fitzgerald E A, and Nayfeh A Theoretical efficiency limit for a two-terminal multi-junction “step-cell” using detailed balance method. Journal of Applied Physics, 2016, 119: 073104.

[23].Dimroth F, Guter W, Schöne J, et al. *Metamorphic GaInP/GaInAs/Ge triple-junction solar cells with≫ 41% efficiency*. in *2009 34th IEEE Photovoltaic Specialists Conference (PVSC)*. 2009. IEEE.

[24].Kufer D and Konstantatos G Highly sensitive, encapsulated MoS2 photodetector with gate controllable gain and speed. Nano letters, 2015, 15: 7307-7313.

[25].Splendiani A, Sun L, Zhang Y, et al. Emerging photoluminescence in monolayer MoS2. Nano Lett, 2010, 10: 1271-5.

[26].Bernardi M, Palummo M, and Grossman J C Extraordinary sunlight absorption and one nanometer thick photovoltaics using two-dimensional monolayer materials. Nano Lett, 2013, 13: 3664-70.

[27].Feng J, Qian X, Huang C-W, et al. Strain-engineered artificial atom as a broad-spectrum solar energy funnel. Nature Photonics, 2012, 6: 866.

[28].Bertolazzi S, Brivio J, and Kis A Stretching and breaking of ultrathin MoS2. ACS Nano, 2011, 5: 9703-9.

[29].Zhang Y, Yang Y, and Wang Z L Piezo-phototronics effect on nano/microwire solar cells. Energy & Environmental Science, 2012, 5: 6850.

[30].Shockley W and Queisser H J Detailed Balance Limit of Efficiency of p-n Junction Solar Cells. Journal of Applied Physics, 1961, 32: 510-519.

[31].Munday J N The effect of photonic bandgap materials on the Shockley-Queisser limit. Journal of Applied Physics, 2012, 112.

[32].Belghachi A, *Theoretical Calculation of the Efficiency Limit for Solar Cells*, in *Solar Cells - New Approaches and Reviews*. 2015.

[33].Rühle S Tabulated values of the Shockley–Queisser limit for single junction solar cells. Solar Energy, 2016, 130: 139-147.

[34].Zhang Y, Liu Y, and Wang Z L Fundamental theory of piezotronics. Adv Mater, 2011, 23: 3004-13.

[35].Duerloo K-A N, Ong M T, and Reed E J Intrinsic Piezoelectricity in Two-Dimensional Materials. The Journal of Physical Chemistry Letters, 2012, 3: 2871-2876.

[36].Zheng D Q, Zhao Z, Huang R, et al. High-performance piezo-phototronic solar cell based on two-dimensional materials. Nano Energy, 2017, 32: 448-453.

[37].Cooper R C, Lee C, Marianetti C A, et al. Nonlinear elastic behavior of two-dimensional molybdenum disulfide. Physical Review B, 2013, 87.

[38].Castellanos-Gomez A, Poot M, Steele G A, et al. Elastic properties of freely suspended MoS2 nanosheets. Adv Mater, 2012, 24: 772-5.

[39].van den Ende D A, van de Wiel H J, Groen W A, et al. Direct strain energy harvesting in automobile tires using piezoelectric PZT–polymer composites. Smart Materials and Structures, 2012, 21.

[40].Wu W, Wang L, Li Y, et al. Piezoelectricity of single-atomic-layer MoS2 for energy conversion and piezotronics. Nature, 2014, 514: 470-4.

[41].Zhou Y, Liu W, Huang X, et al. Theoretical study on two-dimensional MoS2 piezoelectric nanogenerators. Nano Research, 2016, 9: 800-807.

[42].Conley H J, Wang B, Ziegler J I, et al. Bandgap engineering of strained monolayer and bilayer MoS2. Nano letters, 2013, 13: 3626-3630.

[43].Shao R W, Zheng K, Wei B, et al. Bandgap engineering and manipulating electronic and optical properties of ZnO nanowires by uniaxial strain. Nanoscale, 2014, 6: 4936-41.

[44].Akinwande D, Petrone N, and Hone J Two-dimensional flexible nanoelectronics. Nat Commun, 2014, 5: 5678.

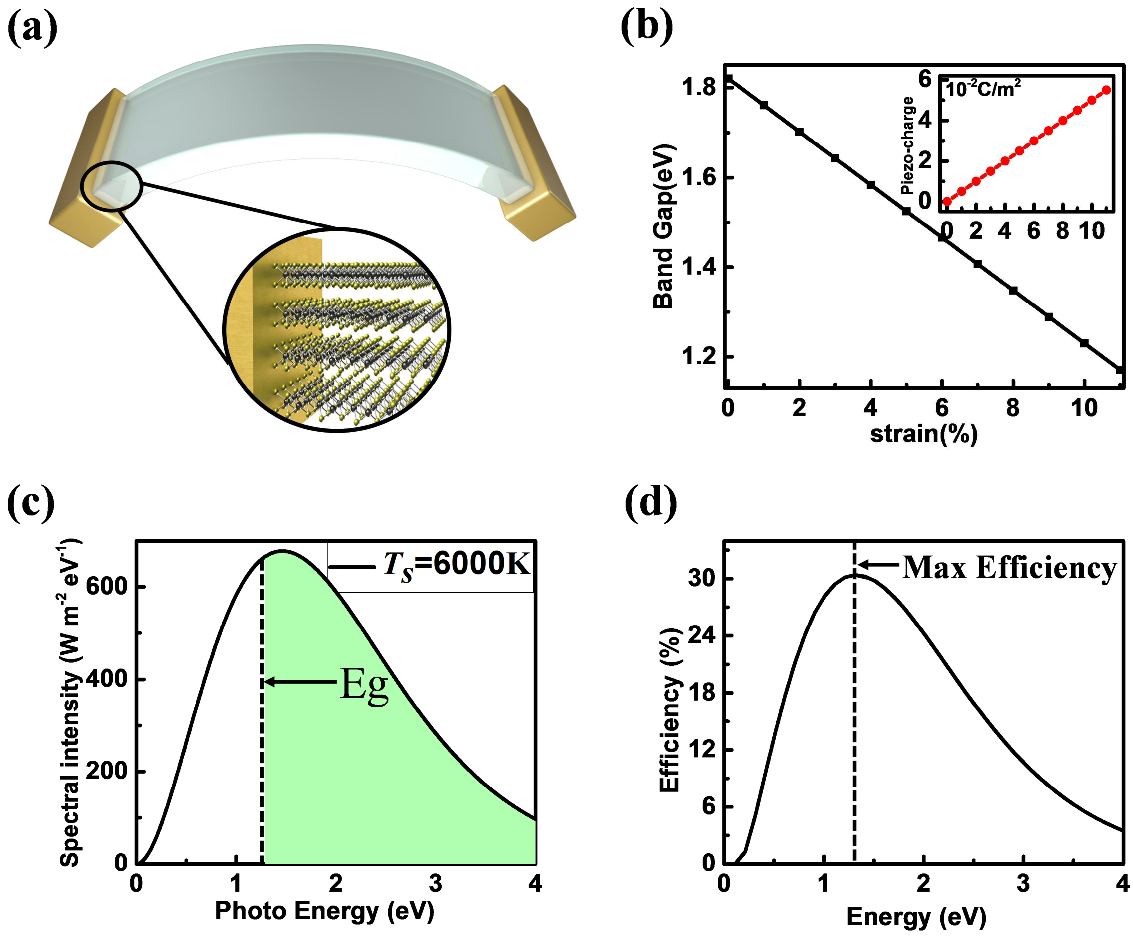
(a)
(b)
1.8
1.6
1.4
1.2
Band Gap(eV)
0
2
4
6
8
10
strain(%)
Piezo-charge
10^{-2}C/m^2
0
2
4
6
(c)
T_S=6000K
Eg
Spectral intensity (W m^{-2} eV^{-1})
0
200
400
600
Photo Energy (eV)
1
3
(d)
Max Efficiency
Efficiency (%)
12
18
24
30
Energy (eV)

Figure 1

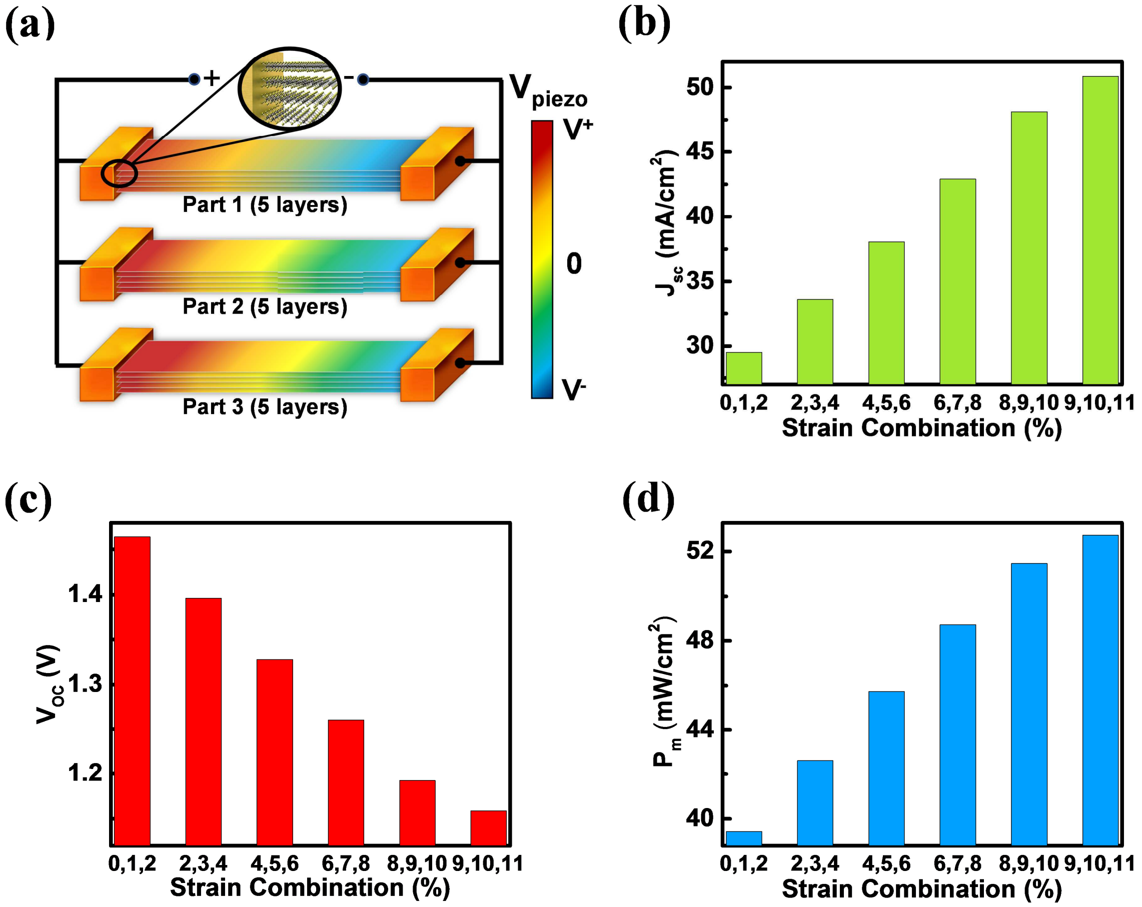
(a)
+
-
V_piezo
V+
0
V-
Part 1 (5 layers)
Part 2 (5 layers)
Part 3 (5 layers)
(b)
J_sc (mA/cm²)
30
35
40
45
50
0,1,2
2,3,4
4,5,6
6,7,8
8,9,10
9,10,11
Strain Combination (%)
(c)
V_oc (V)
1.2
1.3
1.4
0,1,2
2,3,4
4,5,6
6,7,8
8,9,10
9,10,11
Strain Combination (%)
(d)
P_m (mW/cm²)
40
44
48
52
0,1,2
2,3,4
4,5,6
6,7,8
8,9,10
9,10,11
Strain Combination (%)

Figure 2

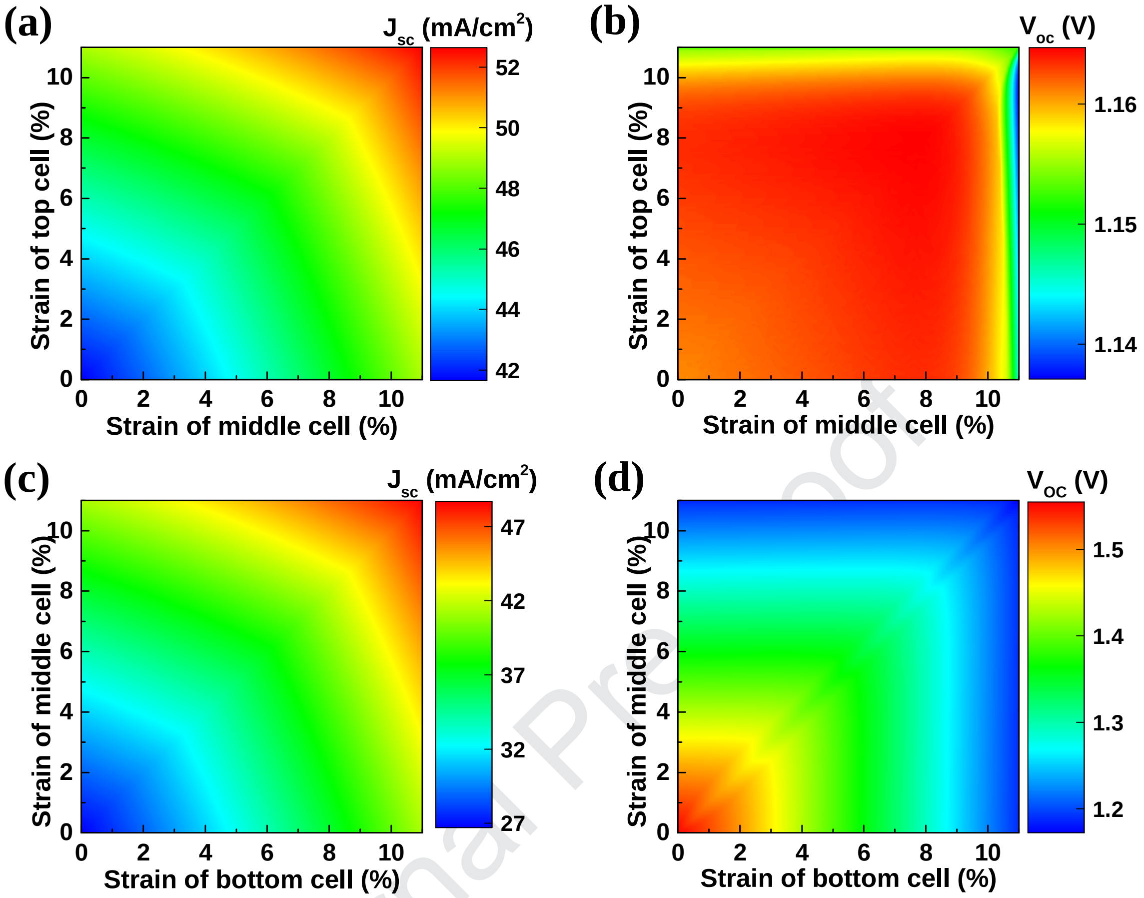
(a)
J_sc (mA/cm²)
52
50
48
46
44
42
Strain of top cell (%)
Strain of middle cell (%)
0
2
4
6
8
10
(b)
V_oc (V)
1.16
1.15
1.14
Strain of top cell (%)
Strain of middle cell (%)
(c)
J_sc (mA/cm²)
47
42
37
32
27
Strain of middle cell (%)
Strain of bottom cell (%)
(d)
V_OC (V)
1.5
1.4
1.3
1.2
Strain of middle cell (%)
Strain of bottom cell (%)

Figure 3

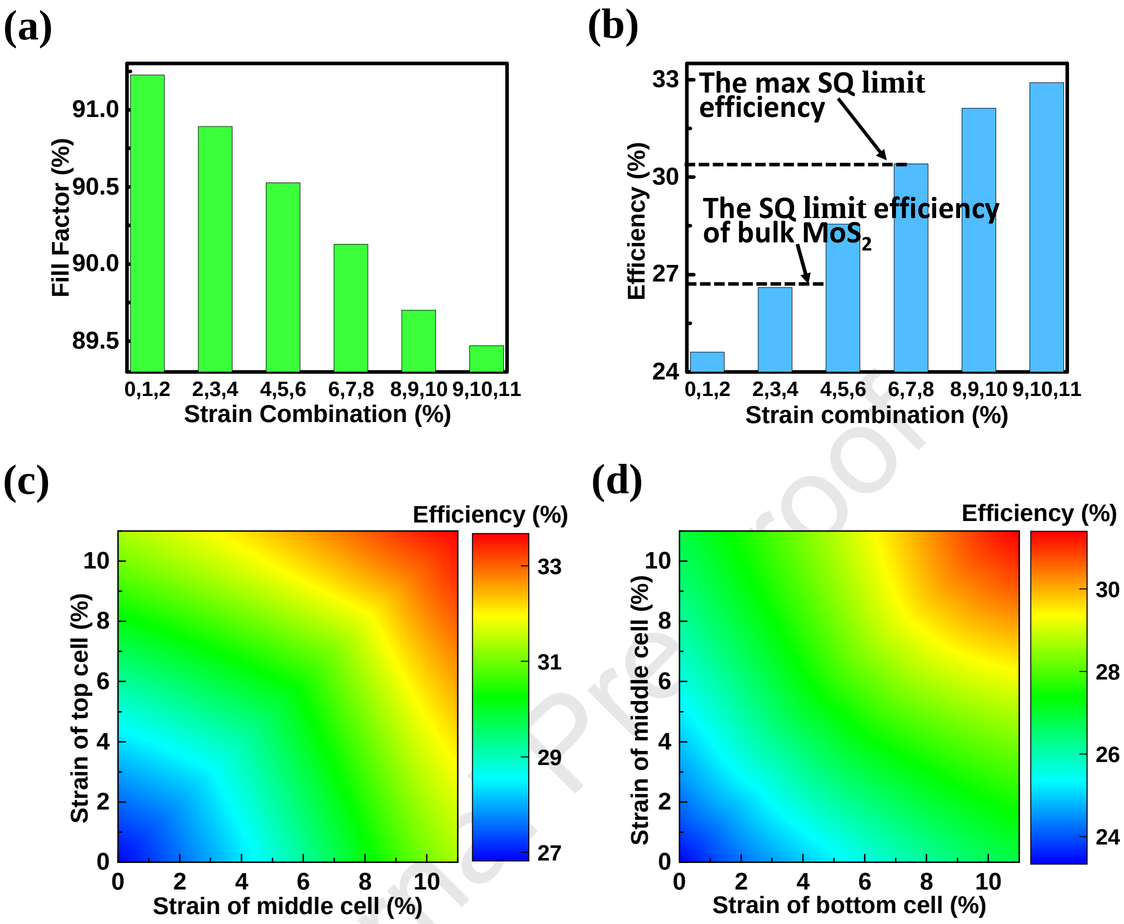
(a)
Fill Factor (%)
91.0
90.5
90.0
89.5
0,1,2
2,3,4
4,5,6
6,7,8
8,9,10
9,10,11
Strain Combination (%)
(b)
Efficiency (%)
33
30
27
24
The max SQ limit efficiency
The SQ limit efficiency of bulk MoS_2
0,1,2
2,3,4
4,5,6
6,7,8
8,9,10
9,10,11
Strain combination (%)
(c)
Efficiency (%)
33
31
29
27
Strain of top cell (%)
0
2
4
6
8
10
Strain of middle cell (%)
(d)
Efficiency (%)
30
28
26
24
Strain of middle cell (%)
0
2
4
6
8
10
Strain of bottom cell (%)

Figure 4

Highlight

1. Piezo-phototronic multijunction solar cell has the potential to break the well-known Shockley–Queisser limit with single-type semiconductor.

2. The efficiency of the piezo-phototronic multijunction solar cell based on MoS_2 reach up to 33%.

3. Piezo-photronics effect enhances power conversion efficiency of piezoelectric semiconductors.

Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.
We confirm that the manuscript has been read and approved by all named authors and that there are no other persons who satisfied the criteria for authorship but are not listed. We further confirm that the order of authors listed in the manuscript has been approved by all of us.
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Signed by all authors as follows:

Yan Zhang Lijie Li Ruhao Liu Gongwei Hu

Jiaheng Nie Yaming Zhang Minjiang Dan Dongqi Zheng

(Michael Gyan)