Unusual properties and potential applications of strain BN-MS\textsubscript{2} (M = Mo, W) heterostructures

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Heterostructures receive intensive attentions due to their excellent intrinsic properties and wide applications. Here, we investigate the natural physical properties and performances of strain BN-MS\textsubscript{2} (M = Mo, W) heterostructure by density functional theory. Different to compressive monolayer MS\textsubscript{2}, corresponding BN-MS\textsubscript{2} heterostructures keep direct band-gap characters because effects of charge transfer on anti-bonding dz\textsuperscript{2} orbitals are stronger than those of Poisson effect. Mexican-hat-like bands without magnetic moments are observed at strain BN-MS\textsubscript{2} heterostructures when the compression is enough. Consequently, electron mobilities of strain BN-MS\textsubscript{2} heterostructures are slightly reduced at first and then enlarged with increasing compressive strain. Note that, strain BN-MS\textsubscript{2} heterostructures reduce the band edges of MS\textsubscript{2} layers and extend their application in photocatalytic water splitting. But just the n-type and p-type schottky barriers of devices with strain BN-MS\textsubscript{2} heterostructures are reduced and even vanished with the increasing tensile and compressive, respectively. Besides, electron mobilities of strain BN-MoS\textsubscript{2} and BN-WS\textsubscript{2} heterostructures can be enhanced to 1290 and 1926 cm\textsuperscript{2} V\textsuperscript{−1} s\textsuperscript{−1}, respectively, with increasing tensile strain. Interestingly, the exciton binding energies of strain BN-MS\textsubscript{2} heterostructures exhibit oscillation variations, different to those of strain monolayer MS\textsubscript{2}.

Two-dimensional transition metal dichalcogenides (TMDs) are an emerging class of materials with atomic thickness, pristine surface, unique and tunable electronic properties which make them highly attractive for applications ranging from nanoelectronics to optoelectronics with high performances\textsuperscript{1,2}. However, many studies have revealed that the performances of nanodevices based on TMDs in experiment are lower than the theoretical expectations\textsuperscript{1–4}. For examples, most measured carrier mobilities of monolayer MoS\textsubscript{2} nanodevices under room temperature are far lower than the theoretical predication of 410 cm\textsuperscript{2} V\textsuperscript{−1} s\textsuperscript{−1}\textsuperscript{5–7}. That can be ascribed to three main reasons: first, the fabricated TMDs flakes in experiment containing several defects, like vacancies, which enhance the scattering effects and deteriorate the intrinsic properties of TMDs\textsuperscript{8,9}. Second, oxide substrates with surface roughness induce strong interfacial charged impurities at substrates-TMDs interfaces\textsuperscript{10–14}. Third, metal-TMDs interfaces usually have large contact resistances and Schottky barrier heights (SBHs) which limit the carrier injection efficiency\textsuperscript{15–19}. To overcome these issues, van der Waals heterostructures engineering, especially BN-TMDs heterostructures, have been employed. Moreover, such approaches have evidently improved the performances of nanodevices based on TMDs. For examples, Wang, \textit{et al.} have fabricated MoS\textsubscript{2}, MoSe\textsubscript{2}, and WS\textsubscript{2} layers on hexagonal boron nitride (BN) substrates to form BN-TMDs heterostructures, which enhanced the photoluminescence and room-temperature mobilities of TMDs due to the reduced substrate traps and improved fake quality\textsuperscript{20–24}. Liao \textit{et al.} have found that forming BN-TMDs heterostructures in metal-TMDs interface regions not only modulated the work function and fermi level pinning effect, but also reduced the SBHs and contacts resistances of metal-TMDs interfaces by an order of magnitude\textsuperscript{25,26}. Moreover, BN-TMDs heterostructures between gate and channel layer could change the main noise source in channel from charged impurities to trapping-detrapping process\textsuperscript{27}. Thus, BN-TMDs heterostructures have been widely used in the high performance nanodevices, including integration\textsuperscript{28}, photoresponse\textsuperscript{29}, self-biased diode\textsuperscript{30}, etc.

It should be noted that MS\textsubscript{2} (M = Mo, W) as typical members of TMDs are not only suitable for above mentioned nanodevices, but also have great potentials in applications of flexible nanodevices, such as flexible battery\textsuperscript{31},...
humidity sensing, flexible supercapacitor, and so on. However, the performances of flexible nanodevices based on MS2, like carrier mobilities, in experiment are far lower than expectation. Moreover, direct-to-indirect transitions occur in band gaps of monolayer MS2 in the flexible nanodevices. Such characters are not conductive to realize high performance flexible nanodevices. Inspired by the excellent performance of BN-TMDs heterostructure in optoelectronics as above mentioned, forming strain BN-MS2 heterostructure with great potential to improve the performance flexible nanodevices. However, few studies have focused on the strain BN-MS2 heterostructures, although the carrier mobilities of monolayer MoS2 flexible transistors had been enlarged from 30 to 45 cm² V⁻¹ s⁻¹ when monolayer MoS2 was substituted by strain BN-MoS2 heterostructure. Moreover, so far few theoretical studies have focused on the natural physical properties of strain BN-MS2 heterostructures. Hence, in this work, the electronic, magnetic, transport, optical properties, and additional potential application of strain BN-MS2 (M = Mo, W) heterostructures were comprehensively investigated by first principles calculations.

### Results and Discussion

#### Geometric structure

Before exploring the strain BN-MS2 (M = Mo, W) heterostructures (Fig. 1a,b), the geometric structures of isolated monolayer BN, MoS2, WS2 were investigated and listed in Table 1. The lattice constants of isolated monolayer BN and MS2 are in good agreement with previous studies. BN-MS2 heterostructures are constructed by stacking the BN and MS2 monolayers on top of each other. To study the natural physical properties of strain BN-MS2 heterostructures accurately, 5×5 BN supercells are constructed and strained to match with the 4×4 MS2 supercells, as shown in Fig. 1. The lattice mismatches of BN-MoS2 and BN-WS2 heterostructures are less than 1%. The equilibrium separations of BN-MoS2 and BN-WS2 heterostructures are 3.28 Å and 3.15 Å, respectively, after extensive test.

#### Electronic properties

To well understand the electronic properties of strain BN-MS2 heterostructures, the electronic structures of corresponding isolated strain monolayer MS2 are studied firstly. Figure 2a as an example...
displays the electronic structure of monolayer MoS$_2$. Monolayer MoS$_2$ is a direct band gap semiconductor with conduction band minimum (CBM) (viz. band A) and valence band maximum (VBM) (viz. band B) at K point. Moreover, its CBM and VBM are mainly dominated by anti-bonding $d_{z^2}$ and bonding $d_{xy}$ orbitals of Mo atoms, respectively. Such characters are consistent with previous reports. In addition, other special bands C, D, and E (marked in Fig. 2a) of monolayer MoS$_2$ are mainly composed of anti-bonding $d_{xy}$, $d_{z^2}$, and bonding $p_{x}$, $p_{y}$ orbitals of S atoms, respectively, as demonstrated in Fig. 2a. Similar characters, except for the band gap, are also observed in monolayer WS$_2$, as shown in Fig. S1. The direct band gaps of monolayer MoS$_2$ and WS$_2$ are 1.76 and 1.91 eV, respectively, which are in accordance with previous reports and listed in Table 1. Note that, although these band gaps are lower than the experimental values, they are closer to the transport band gaps in nanodevices compared to the band gap calculated by GW and HSE functional. That is because the strong Coulombic screening by metal electrodes can minimize the exciton binding energies and many body effects of 2D materials. Moreover, the electronic structures of MoS$_2$ calculated by PBE functional are similar to those calculated by HSE functional (as demonstrated in Fig. S2). It suggests that PBE functional is sufficient to study the electronic properties of MoS$_2$ layers and BN-MoS$_2$ heterostructures.

When monolayer MoS$_2$ undergoes tensile strain, the band gap reduces gradually and accompanied with a direct-to-indirect band gap transition. That is because the thickness of MoS$_2$ (as listed in Table 1) is reduced by tensile strains due to the Poisson effect. Such thickness reduction strengthens the coupling between the $p_x$ orbitals of S atoms and $d_{z^2}$ orbitals of M atoms, and such biaxial tensile strain weakens the coupling between the $p_x + p_y$ orbitals of S atoms and $d_{xy}$ orbitals of M atoms. As a result, the energies of anti-bonding band A and bonding band B reduce, and the energies of anti-bonding bands C and bonding band D enlarge. Consequently, the VBM shifts up and moves from K to $\Gamma$ point, and the CBM at the K point shifts down, leading to the reduction of band gaps with increasing tensile strain, as shown in Fig. 2b. On the contrary, application of compressive strain enlarges the thickness of monolayer MoS$_2$, and then weakens the coupling between the $p_x + p_y$ orbitals of S atoms and $d_{xy}$ orbitals of M atoms and enhances coupling between the $p_x + p_y$ orbitals of S atoms and $d_{z^2}$ orbitals of M atoms. Consequently, the anti-bonding bands A and C shift up and down, respectively. The position of CBM transforms from anti-bonding band A to anti-bonding band C, leading to a direct-to-indirect transition, as shown in Fig. 2c. Nevertheless, it should be noted that the energy of anti-bonding band C is higher than that of anti-bonding band A of monolayer MoS$_2$ without strain, and it decreases slightly with the increasing compressive strain. As a result, the energy of band C of monolayer MoS$_2$ with small compressive strain is still higher than that of band A of monolayer MoS$_2$ without strain. Thus, the band gaps of monolayer MoS$_2$ slightly enlarge at first and then decrease with the increasing enlarge compressive strain, as displayed in Fig. 3a, which is consistent with previous reports. In addition, the enhanced coupling between the $p_x + p_y$ orbitals of S atoms and $d_{z^2}$ orbitals of M atoms induced by compressive strain also rises the energy of bonding band E, as shown in Fig. 2c. When the compressive strain is larger than 8%, such raised bonding band E can surpass that of raised bonding band B. Consequently, the position of VBM shifts from the bonding band B at the K point to bonding band E at the M point, leading to a direct-to-indirect transition, as shown in Fig. 2d.

Figure 2. Projected band structures of monolayer MoS$_2$ (a) without strain, and with (b) 4% tensile, (c) 4% compressive and (d) 10% compressive strains, respectively. Projected band structures of BN-MoS$_2$ heterostructures (e) without strain, and with (f) 4% tensile, (g) 4% compressive and (h) 12% compressive strains, respectively. The insertions in (g) and (h) are the conduction bands around the K points.
For BN-MS₂ heterostructures, their CBM and VBM are dominated by the MS₂ layer, such as the BN-MoS₂ heterostructure in Fig. 2e. Moreover, the components and positions of CBM and VBM of BN-MS₂ heterostructures are similar to those of monolayer MS₂. It suggests that the intrinsic electronic properties can be remained when monolayer MS₂ transforms to type-I BN-MS₂ heterostructure. However, the band gaps reduce slightly to be 1.72 and 1.88 eV for BN-MoS₂ and BN-WS₂ heterostructures, respectively. That is because the weak charge transfer between BN and MS₂ layers (as shown in Fig. S3) slightly reduce the anti-bonding band A. When BN-MS₂ heterostructures undergo tensile strain, they keep type-I heterostructure characters, and their CBM and VBM are still dominated by MS₂ layer. Moreover, variations of band gaps and band edges of tensile BN-MS₂ heterostructures (see Fig. 2f) are similar to those of tensile monolayer MS₂ although the biaxial tensile also induces the reduction of MS₂ layer thickness in BN-MS₂ heterostructures (as listed in Table 1). However, the reduction indirect band gaps of tensile BN-MS₂ heterostructures are slightly lower than those of corresponding tensile monolayer MS₂, as exhibited in Fig. 3a. That is because additional charges are accumulated at the MS₂ layer of BN-MS₂ heterostructures (as displayed in Fig. S3), which can further reduce the energy of anti-bonding dₓ²−ᵧ² orbits. Hence, the energy of anti-bonding band C is still higher than that of anti-bonding band A at the K point which dominates the CBM of BN-MS₂ heterostructure. It should be noted that, except for the Poisson effect induced by compressive strain, the wrinkle phenomenon is also introduced to the MS₂ layer of BN-MS₂ heterostructure as the compressive strain continue to increases, which induce a heterogeneous charge transfer between BN and MS₂ layers of BN-MS₂ heterostructures (as displayed in Fig. S4). As a result, the energy of anti-bonding orbitals dₓ²−ᵧ² + dᵧ² is close to that of anti-bonding orbitals dₓ², and a Mexican-hat-like band around K point is formed, as shown in Fig. 2g.h. In general, the Mexican-hat-bands suggesting an obviously magnetic moments. Nevertheless, nonmagnetic states are observed for BN-TMDs with larger compressive strain, as displayed in Fig. S5. When the compressive strain continues enlarging, such a Mexican-hat-like band becomes more evident, and a direct-to-indirect band gap transition is
observed, as displayed in Fig. 2h. That is because the weak interaction is insufficient to hamper the increasing energy of the bonding band E at the M point.

**Band levels and applications.** Figure 3b displays the band edges of BN-MS2 heterostructures and monolayer MS2 on an absolute energy scale with respect to the vacuum level. For monolayer MS2, their band edges of VBM and CBM states of monolayer MoS2 and WS2 are −5.97, −4.18 eV and −5.56, −3.63 eV, respectively, which are consistent with previous reports. The VBMs are enhanced with both the increasing compressive and tensile strains since compressive and tensile strain can enhance the bonding band B and bonding band D, respectively. The CBMs reduce monotonously with the increasing tensile strain, while they enlarge at first and then reduce with the increasing compressive strain due to the transfer of CBM due to the transformation of CBM, as above analysis. For strain BN-MS2 heterostructures, similar characters are observed. Nevertheless, the band edges of BN-MS2 heterostructures are lower than those of corresponding MS2 due to the charge transfer between BN and MS2 layer, as above analysis.

It is well known that the band levels are related to the applications in photocatalytic and electronic fields. Figure 3c demonstrates the schematic of photocatalytic water splitting. A good photocatalytic material for water-splitting requires that the CBM and VBM are lower and higher than the reduction and oxidation potentials of water, respectively. Thus, monolayer WS2 is not a good photocatalytic material, as displayed in Fig. 3b. However, the CBM and VBM of BN-WS2 heterostructures are higher and lower than reduction and oxidation potentials of water, respectively. Moreover, such characteristics remain when the compressive and tensile strains of BN-WS2 heterostructures are lower than 2%. In other words, forming BN-WS2 heterostructures can extend the application of monolayer WS2 in the photocatalytic water splitting. For the monolayer MoS2, its band edges are outside of the reduction and oxidation potentials of water when compressive strain is lower than 4%. It means that monolayer MoS2 may be suitable for the application of photocatalytic water splitting, but the compressive strain is limited to be 4%. Upon forming BN-MoS2 heterostructure, similar characters can be observed when the compressive strain is up to 6%. It suggests that forming BN-MoS2 heterostructures can extend the application of strain monolayer MoS2 in photocatalytic water splitting.

Figure 3d displays the schematic diagrams of metal/semiconductor contacts in FETs which is usually used to calculate ideal SBH values according to Schottky–Mott rule without Fermi level pinning. For metal/MS2 contacts with strong Fermi level pinning effects, their large SBHs are difficult to be obtained by such methods, and they are difficult to be reduced and vanished by strained monolayer MS2. Different to metal/MS2 contacts, metal/MoS2 contacts with BN-MoS2 heterostructures show negligible Fermi level pinning effect. The SBHs at metal/MoS2 contacts with strain BN-MS2 heterostructures can be obtained directly from the difference between band levels heterostructures and work functions (WFs) of metal electrodes. Figure 3e as an example shows the relationship between the WFs of metal and strain BN-MoS2 heterostructure. No matter what the work function of metal electrode, the n-type and p-type SBHs reduce with the increasing tensile and compressive strain of BN-MoS2 heterostructures, respectively. The detailed variations of SBHs of metal/MoS2 contacts induced by strained BN-MoS2 heterostructures are displayed in Fig. 3f. The ideal n-type SBHs of Ti/MoS2 and Ag/MoS2 contacts with BN-MoS2 heterostructures are −0.02 and 0.20 eV, respectively, which are lower than those of pure metal/MoS2 contacts. When BN-MoS2 heterostructures undergo tensile strain, these n-type SBHs continue reducing and even vanishing, as exhibited in Fig. 3f. For example, the lowest n-type SBHs of Ti/MoS2 and Ag/MoS2 contacts with tensile BN-MoS2 heterostructures are low to −1.04 and −0.83 eV, respectively. In addition, the p-type SBH of Pt/MoS2 contact with BN-MoS2 heterostructure is about 0.19 eV which is far lower than that of pure Pt/MoS2 contact. Moreover, such p-type SBH can be further vanished when the compressive strain is larger than 2%, as shown in Fig. 3f. As to metal/WS2 contacts with strain BN-WS2 heterostructures, similar characteristics are also found, as displayed in Fig. 3f. Such results indicate that substituting strain monolayer MS2 in flexible devices by strain BN-MS2 heterostructures can realize high performance MS2 devices with low contact properties.

**Transport properties.** Figure 4 gives the carrier effective masses and room-temperature mobilities of strained monolayer MS2 and BN-MS2 heterostructures. For monolayer MS2, the electron and hole mobilities at room-temperature of monolayer MoS2 and WS2 are 77.17, 155.79 cm2 V−1 s−1, and 163.22, 651.56 cm2 V−1 s−1, respectively, and the effective electron and hole masses of monolayer MoS2 and WS2 are 0.48, 0.64 m0 and 0.30, 0.38 m0, respectively, which are in good agreement with previous reports. These effective electron masses reduce because either compressive or tensile strains are added to monolayer MS2. These effective hole masses enhance at first and then reduce with the increasing tensile strain since the position of VBM occurs a K-to-Γ transition; while they enlarge monotonically with the increasing compressive strain. That is because a K-to-M transition occurs at the position of VBM and the compressive strain is lower than 8%. In general, the small effective mass indicates the large carrier mobility. As a result, the variations of electron and hole mobilities of strain monolayer MS2 are opposite to those of corresponding effective masses, as exhibited in Fig. 4. In other words, both compressive and tensile strains can enlarge the electron mobilities of monolayer MS2. It should be noted that, nevertheless, the experimental electron mobilities of strain monolayer MS2 in flexible nanodevices are lower than those of monolayer MS2, due to the interfacial charged impurities induced by Si/SiO2 substrates with large surface roughness.

For BN-MS2 heterostructures, the effective electron and hole masses of BN-MoS2 and BN-WS2 heterostructures are 0.47, 0.57 m0 and 0.28, 0.37 m0, respectively, which are slightly lower than those corresponding values of monolayer MS2. It means higher carrier mobilities for BN-MS2 heterostructures compared to monolayer MS2. The enhanced electron and hole mobilities of BN-MoS2 and BN-WS2 heterostructures are 223.50, 213.20 cm2 V−1 s−1, and 505.04, 751.63 cm2 V−1 s−1, respectively. When BN-MS2 heterostructures undergo tensile strain, their effective electron masses are lower than those of corresponding tensile monolayer MS2. An opposite phenomenon
occurs for BN-MS2 heterostructures with compressive strain. Moreover, different to monolayer MS2, the effective electron masses of BN-MS2 heterostructures reduce monotonically with the increasing tensile strain, while they enlarge at first and then reduce with the increasing compressive strain since the increased compressive strain induces the formation of a Mexican-hat-like band gradually. As a result, the enhanced room-temperature electron mobilities of BN-MS2 heterostructures can be further enlarged with the increasing tensile strain, and are higher than those of corresponding monolayer MS2; while they reduce at first and then enlarge with the increasing compressive strain. It should be noted that the lowest electron mobilities of BN-MS2 heterostructure are close to that of monolayer MS2, although the electron mobilities of compressive BN-MS2 heterostructure are lower than those of corresponding compressive MS2, as shown in Fig. 4a,c. For examples, the lowest electron mobility of BN-MoS2 heterostructure of about 56.48 cm² V⁻¹ s⁻¹ is close to that of monolayer MS2 of about 77.16 cm² V⁻¹ s⁻¹. In addition, BN layer without dangling bonds can strongly weaken the interfacial charged scattering. Such characters suggest that flexible nanodevices based on BN-MS2 heterostructures can obtain higher electron mobilities than MS2 flexible nanodevices in experiment.  

Optical properties. Except for the transport properties, the variations of effective masses can also modulate the exciton binding energies. The calculated exciton binding energies of monolayer MoS2 and WS2 are about 0.98 and 0.61 eV, respectively, which are close to previous studies. Moreover, these exciton binding energies enlarge at first and then reduce as the strain changes from compressive to tensile. Upon forming the BN-MoS2 and BN-WS2 heterostructures, the exciton binding energies are enhanced 1.05 and 0.65 eV, respectively, because MS2 layers accept charges from BN layers, as shown in Fig. S3. Interestingly, the exciton binding energies of strain BN-MS2 heterostructures exhibit oscillation variation, just like a “M”, as demonstrated in Fig. 5a. In addition, the absorption coefficients of strain BN-MS2 heterostructures are enlarged compared to those monolayer MS2, no matter what strains are added to monolayer and BN-MS2 heterostructures, as the examples illustrated in Fig. 5b.

Conclusion
In summary, electronic and optical properties of strain monolayer MS2 and BN-MS2 heterostructures and their potential performance are comprehensively investigated by density functional theory. All strain BN-MS2 heterostructures are type-I heterostructures, irrespective of compressive and tensile strain. However, different to the indirect band gap characters of compressive monolayer MS2, corresponding compressive BN-MS2 heterostructures keep direct band gap characters because effects of charge transfer on anti-bonding dₓz orbitals are stronger than those of Poisson effect. Moreover, Mexican-hat-like bands without magnetic moments are observed for
compressive BN-MS₂ heterostructures due to the non-uniform charge transfer induced by wrinkle. Consequently, electron mobilities of flexible devices with BN-MS₂ heterostructures are reduced at first and then enlarged with the increasing compressive strain, different to those of compressive monolayer MS₂. In addition, although strain can induce similar variations of band edges between BN-MS₂ heterostructures and monolayer MS₂ and extend their application in photocatalytic water splitting, strain just can reduce the Schottky barriers of devices with BN-MS₂ heterostructures. Moreover, the n-type and p-type Schottky barriers are reduced and even vanished with the increasing tensile and compressive strain, respectively. For tensile BN-MS₂ heterostructures, variations of their transport properties are similar to those of monolayer MS₂, except for higher electron and hole mobilities and lower effective electron and hole masses. The room-temperature electron mobilities of MoS₂ and WS₂ layers in tensile BN-MS₂ heterostructures can be up to 1290 and 1926 cm² V⁻¹ s⁻¹, respectively. In addition, the exciton binding energies of strain BN-MS₂ heterostructures exhibit oscillation variations, different to those of strain monolayer MS₂.

Computational Methodology

All calculations were performed within first-principles density functional theory (DFT) using projector augmented-wave (PAW) pseudopotentials, as implemented in the Vienna Ab Initio Simulation Package (VASP). The Generalized Gradient Approximation (GGA) parameterized by Perdew-Burke-Ernzerhof (PBE) was employed to adopt for the exchange-correction functional. The van der Waals (vdW) interactions were considered using the method of Grimme (D2). The cut-off energy was set to be 450 eV. The convergence criterions were 1 × 10⁻⁶ eV for the self-consistent field energy and 0.01 eV/Å for the residual forces on each atom, respectively. The Monkhorst-Pack k-point mesh was sampled with a separation of about 0.015 Å⁻¹ in the Brillouin zone during the relaxation and electronic calculation periods. To minimize the interlayer interactions under the periodic boundary condition, vacuums of 15 Å were added perpendicular to the layer planes of heterostructure.

The carrier mobilities were calculated by the following expression,

\[ \mu = \frac{2e\hbar^3C}{3k_B^2T E^2 m^*} \]

where \( \hbar \) is the Planck constant, \( k_B \) is Boltzmann constant, \( T \) is the temperature (set to be 300 K), \( m^* \) is the effective mass which is calculated by \( m^* = \hbar^2 / \left[ \partial^2 \mathcal{E}(k) / \partial k^2 \right]^{-1} \), \( E \) is the deformation potential constant which denotes the shift of the band edges induced by strain. \( C \) is the elastic modulus of a uniformly deformed crystal for simulating the lattice distortion activated by the strain, defined by \( C = [\partial^2 \mathcal{E} / \partial \delta^2] / S_0 \) where \( \mathcal{E} \) is the total energy of the supercell, \( \delta \) is the applied uniaxial strain, and \( S_0 \) is the area of the optimized supercell.

All the exciton binding energies of monolayer MS₂ and BN-MS₂ heterostructures were calculated by adopting the simplified hydrogen-like Wannier-Mott exciton modes,

\[ E_b = \mu_{ex} R_y \varepsilon_r^2 / m_e \]

where \( E_b \) is the excitation binding energy, \( \mu_{ex} = m_e \times m_h / (m_e + m_h) \), \( m_e \) and \( m_h \) are the effective electron and hole masses, respectively, \( R_y \) is the atomic Rydberg energy, and \( \varepsilon_r \) is the relative dielectric constant.

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**Acknowledgements**

This work was financially supported by the National Natural Science Foundation of China (Grant 61604119, 61704131, and 61804111); Natural Science Foundation of Shaanxi Province (Grant 2017JQ6002, and 2017JQ6031); Initiative Postdocs Supporting Program (Grant BX20180234); Project funded by China Postdoctoral Science Foundation (Grant 2018M643578); Fund of the State Key Laboratory of Solidification Processing in NWPU (Grant SKLSP201857). The 111 Project (Grant B12026). The numerical calculations in this paper have been done on the HPC system of Xidian University.

**Author Contributions**

The idea was conceived by J.S., J.C. and J.Z. The simulation was performed by J.H. and J.Z. The data analyses were performed by J.S., Z.L., J.C. and Y.H. Tis manuscript was written by J.S., Z.L. and J.C. All authors discussed the results and contributed to the paper.

**Additional Information**

Supplementary information accompanies this paper at https://doi.org/10.1038/s41598-019-39970-0.

**Competing Interests:** The authors declare no competing interests.

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