First principles calculations of the interface properties of amorphous-$\text{Al}_2\text{O}_3$/MoS$_2$ under non-strain and biaxial strain conditions

Li-Bin Shi, Ming-Biao Li, Xiao-Ming Xiu, Xu-Yang Liu, Kai-Cheng Zhang, Yu-Hui Liu, Chun-Ran Li, and Hai-Kuan Dong

School of Mathematics and Physics, Bohai University, Liaoning Jinzhou 121013, China

(Dated: 22 February 2017)

$\text{Al}_2\text{O}_3$ is a potential dielectric material for metal-oxide-semiconductor (MOS) devices. $\text{Al}_2\text{O}_3$ films deposited on semiconductors usually exhibit amorphous due to lattice mismatch. Compared to two-dimensional graphene, MoS$_2$ is a typical semiconductor, therefore, it has more extensive application. The amorphous-$\text{Al}_2\text{O}_3$/MoS$_2$ (a-$\text{Al}_2\text{O}_3$/MoS$_2$) interface has attracted people’s attention because of its unique properties. In this paper, the interface behaviors of a-$\text{Al}_2\text{O}_3$/MoS$_2$ under non-strain and biaxial strain are investigated by first principles calculations based on density functional theory (DFT). First of all, the generation process of a-$\text{Al}_2\text{O}_3$ sample is described, which is calculated by molecular dynamics and geometric optimization. Then, we introduce the band alignment method, and calculate band offset of a-$\text{Al}_2\text{O}_3$/MoS$_2$ interface. It is found that the valence band offset (VBO) and conduction band offset (CBO) change with the number of MoS$_2$ layers. The dependence of leakage current on the band offset is also illustrated. At last, the band structure of monolayer MoS$_2$ under biaxial strain is discussed. The biaxial strain is set in the range from -6% to 6% with the interval of 2%. Impact of the biaxial strain on the band alignment is investigated.

PACS numbers: 68.35.-p, 77.55.D-, 77.80.bn

I. INTRODUCTION

Since integrated circuit was born in 1958, the microelectronic technology has made rapid development. Moore’s law predicts that the number of metal-oxide-semiconductor-field-effect-transistors (MOSFETs) on a chip doubles every 18 months. For a long time, the gate oxide of integrated circuit has been using silicon dioxide. In order to further reduce the feature size of integrated circuits, we must abandon silicon dioxide, and select the materials with higher relative dielectric constant (high-$\kappa$)\cite{1}. If high-$\kappa$ materials are used to replace conventional silicon dioxide as the gate dielectric material, the physical thickness of the gate dielectric layer can be increased, so that the gate leakage current can be greatly suppressed. In order to develop field effect transistors with lower power consumption and higher efficiency, people have done a lot of research on high-$\kappa$ materials, including $\text{Ta}_2\text{O}_5$\cite{2}, $\text{Si}_3\text{N}_4$\cite{3}, $\text{Gd}_2\text{O}_3$\cite{4}, $\text{La}_2\text{O}_3$\cite{5}, $\text{Y}_2\text{O}_3$\cite{6}, $\text{Sc}_2\text{O}_3$\cite{7}, $\text{Ga}_2\text{O}_3$\cite{8}, $\text{Lu}_2\text{O}_3$\cite{9}, $\text{Al}_2\text{O}_3$\cite{10,11}, $\text{LaAlO}_3$\cite{12}, $\text{SrTiO}_3$\cite{13}, $\text{LaLuO}_3$\cite{14,15}, $\text{ZrO}_2$\cite{16,17}, $\text{HfO}_2$\cite{18,19}, Hf silicate\cite{20} and Zr silicate\cite{21} $\text{Al}_2\text{O}_3$ among them has become a promising candidate due to its larger band gap (5–9 eV) and moderate dielectric constant (8–10).

$\text{Al}_2\text{O}_3$ thin films deposited on semiconductor substrates usually display amorphous due to lattice mismatch between $\text{Al}_2\text{O}_3$ and semiconductors\cite{22,23}. Amorphous-$\text{Al}_2\text{O}_3$ (a-$\text{Al}_2\text{O}_3$) has a complex structure, and knowledge of its microstructure plays an important role in the analysis of the oxidation and passivation details of aluminum. A-$\text{Al}_2\text{O}_3$/semiconductor interface is expected to be superior to crystalline-$\text{Al}_2\text{O}_3$/semiconductor interface due to lower interface defect density. At present, a large number of theoretical and experimental studies have been done on crystalline $\text{Al}_2\text{O}_3$\cite{24,25} which mainly include the crystal structure, defect formation and electronic structure. There is not much research on a-$\text{Al}_2\text{O}_3$ as a dielectric due to the complex microscopic structure. In particular, there is less theoretical research on the formation mechanism of a-$\text{Al}_2\text{O}_3$.

Since the discovery of graphene in 2004, two-dimensional materials have attracted people’s attention\cite{26,27}. Low dimensional materials are interesting not only because they can provide access to novel physical phenomena, but also because their unique electrical, optical and mechanical properties make them the focus of attention. $\text{MoS}_2$ crystal is composed of Mo atomic layer sandwiched between two layers of S, forming a triangular prismatic arrangement\cite{28,29}. The Mo-S bonding is strong covalent, but the coupling between MoS$_2$ monolayer is weak van der Waals interactions. Because monolayer MoS$_2$ is a typical semiconductor, it is considered as promising candidates for nanoelectronics applications. However, one of the major limiting factors for low dimensional materials is the interface. At present, people have done some research on $\text{Al}_2\text{O}_3$ and MoS$_2$\cite{30,31}. However, the $\text{Al}_2\text{O}_3$/MoS$_2$ interface properties are paid little attention. We have not found a detailed study of the a-$\text{Al}_2\text{O}_3$/MoS$_2$ interface under biaxial strain.

In this paper, we have done three aspects of studies. First, we investigate generation of a-$\text{Al}_2\text{O}_3$ by first principles molecular dynamics simulations. Then, we analyze band alignment between a-$\text{Al}_2\text{O}_3$ and MoS$_2$. Impact
of the MoS$_2$ layer thickness on band offset is discussed. At last, we investigate effects of the biaxial strain on a-Al$_2$O$_3$/MoS$_2$ interface. Impact of the band offset on leakage current is discussed.

II. COMPUTATIONAL DETAILS

A. Generation of amorphous-Al$_2$O$_3$ sample

Amorphous-Al$_2$O$_3$ is generated by melting and quenching technique. Molecular dynamics with NVT ensemble and geometric optimization based on density functional theory (DFT) are performed in the calculation. Generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) is choose as exchange correlation functional during molecular dynamics simulation. All calculations are carried out in CASTEP code based on the total-energy pseudopotential method.[1]

Figure 1 describes the specific generation process of a-Al$_2$O$_3$ sample. It is prepared by starting with a monoclinic crystal corresponding to $\theta$-Al$_2$O$_3$ at the density of 3.61 g/cm$^3$, which is presented in Fig. 1 (a). Its lattice constants are $a=11.80\,\text{Å}$, $b=2.91\,\text{Å}$, and $c=5.62\,\text{Å}$. In order to perform molecular dynamics simulations, we cut $\theta$-Al$_2$O$_3$ along (100) direction, and construct a orthogonal Al$_2$O$_3$ supercell by $3 \times 2 \times 1$ extension. The supercell consists of 72 O and 48 Al atoms with lattice constants of $a=8.73\,\text{Å}$, $b=11.24\,\text{Å}$, and $c=11.50\,\text{Å}$, which is shown in Fig. 1(b). High temperature annealing at low density provides very good oxide mixing and completely removes the original ordered geometry. The low density sample is formed by rescaling the supercell box size along every direction. In order to ensure the full mixing between the oxides, we construct the low density Al$_2$O$_3$ sample with value of 0.62 g/cm$^3$ by expanding the supercell box size 1.8 times. Fig. 1 (c) presents the sample prepared by annealing at 5000 K for 1 ps with time step of 1 fs. In order to obtain experimental results, we must gradually increase the sample density. We first increase the sample density to 1.32 g/cm$^3$ by rescaling the supercell box size from 1.8 times to 1.4 times, subsequent sample is annealed at 5000 K for 0.5 ps with time step of 1 fs. Fig. 1 (d) shows the sample after annealing at 5000 K. Then, the sample density is increased to 2.37 g/cm$^3$ by rescaling the supercell box size from 1.4 times to 1.15 times. Fig. 1 (e) shows the sample annealed at 5000 K for 0.5 ps with time step of 1 fs. Finally, we increase the sample density to 3.4 g/cm$^3$ by rescaling the supercell box size, which is in agreement with experimental values of 3.05 g/cm$^3 \sim 3.40$ g/cm$^3$ for a-Al$_2$O$_3$ sample. The sample is annealed at 5000 K for 0.5 ps with time step of 1 fs, and quickly cooled up to 10 K. Fig. 1 (f) presents the cooled sample. In order to eliminate the internal stress, we do geometric optimization on samples, which is shown in Fig. 1 (g).

The electronic structure analysis for the annealed and relaxed a-Al$_2$O$_3$ indicates a band gap of 3.66 eV, which is in agreement with a previous DFT band gap of 3.80 eV. It is well known that the GGA underestimate band gaps of semiconductors or oxides, which leads to inaccurate calculations of band alignments. The hybrid Heyd-Scuseria-Ernzerhof functional (HSE) combines screened Hartree Fock exchange with the GGA-PBEalsa functionals. The results indicate that the values calculated by HSE functional are close to previous simulations and experiments. Our results are found to be very close to previous simulations and experiments, which indicates that our a-Al$_2$O$_3$ sample is close to the actual situation.
B. Band alignment methods

One of the most important features on oxide/semiconductor interfaces is band offset, i.e., the relative energy level positions on both sides of the interface. The valence band offset (VBO) can be defined as the difference between positions of valence band maximum (VBM), which can be obtained by calculating the band structure and average electrostatic potential (AEP). In the potential line up method, the VBO is usually split into two terms:

\[ \text{VBO} = \Delta E_v + \Delta V \]  

(1)

The first contribution of $\Delta E_v$ corresponds to alignment of VBM for bulk band structure term of oxide and semiconductor. The second term of $\Delta V$ corresponds to the macroscopic AEP alignment, which can be determined by two methods. One method is to determine the macroscopic AEP by constructing the oxide/semiconductor interface. The other is to determine the macroscopic AEP by constructing oxide and semiconductor surfaces. $\text{SrTiO}_3/\text{TiO}_2$ interface has been extensively investigated because the in-plane lattice mismatch between $\text{SrTiO}_3$ and $\text{TiO}_2$ along (001) direction is less than 3%. In order to verify the validity of two methods, we calculate the VBO by constructing $\text{SrTiO}_3$ and $\text{TiO}_2$ surfaces as well as $\text{SrTiO}_3/\text{TiO}_2$ interface. It is found that the surface and interface calculations can give similar results, which is also found in previous investigation of $\text{Al}_2\text{O}_3$/III-V interface.\(^{25}\) The VBO calculated by constructing material surface is similar to that calculated by calculating the work function of the material, which has been widely used to study the band offset.\(^{38,66}\)

In this paper, we align the macroscopic AEP by constructing $\alpha\text{-Al}_2\text{O}_3$ and $\text{MoS}_2$ surfaces instead of $\alpha\text{-Al}_2\text{O}_3$ sample.
The vacuum level is scaled to zero. Macroscopic AEP is planar and macroscopic AEP. In order to align the AEP, slightly overestimated by HSE. The band gap is underestimated by GGA-PBE while it is Comparing to the experimental values, it is found that the value of band gap for monolayer MoS\(_2\) is 1.90 eV. Therefore, it is noted that the VBM position moves upward as the number of MoS\(_2\) layers is increased.

III. RESULTS AND DISCUSSION

A. Band alignment of a-Al\(_2\)O\(_3\)/MoS\(_2\) interface

In order to elucidate band gap shift, we calculate the band structures for bulk and different thickness layers of MoS\(_2\) by GGA-PBE and HSE functionals as shown in Fig. 2. The band structures suggest that bulk MoS\(_2\) is a semiconductor with indirect band gap, the VBM at G-point, and the conduction band minimum (CBM) between K-point and G-point. This calculation is consistent with previous investigation.\(^{39}\) Calculated band gap is 0.98 eV for GGA-PBE and 1.46 eV for HSE. It is found that HSE band gap is close to experimental value of 1.30 eV.\(^{37}\) For 4-layer MoS\(_2\), the band gap is increased to 1.06 eV for GGA-PBE and 1.54 eV for HSE. We are surprised to find that the CBM shifts to K-point as MoS\(_2\) changes from bulk structure to 4-layer MoS\(_2\). However, the positions of VBM can not be found to change significantly. It is noted that the band gap increases with the decrease of the number of MoS\(_2\) layers. The GGA-PBE and HSE band gap increases to 1.09 eV and 1.58 eV for 3-layer MoS\(_2\), and 1.19 eV and 1.69 eV for 2-layer MoS\(_2\). Interestingly, the position of VBM shifts from G-point to K-point as MoS\(_2\) changes from 2-layer MoS\(_2\) to 1-layer MoS\(_2\) (monolayer MoS\(_2\)). Therefore, it changes from indirect gap semiconductor to direct band gap semiconductor. The GGA-PBE and HSE band gap increase to 1.63 eV and 2.11 eV for 1-layer MoS\(_2\). The experimental value of band gap for monolayer MoS\(_2\) is 1.90 eV.\(^{37}\) Comparing to the experimental values, it is found that the band gap is underestimated by GGA-PBE while it is slightly overestimated by HSE.

Figure 3 shows a-Al\(_2\)O\(_3\) and MoS\(_2\) surfaces as well as planar and macroscopic AEP. In order to align the AEP, the vacuum level is scaled to zero. Macroscopic AEP is the averaged value of planar AEP, which is represented by a red point connection in Fig. 03. For MoS\(_2\) surface, the planar AEP in the atomic region exhibits a periodic oscillation, while it remains constant in the vacuum region.\(^{67}\) It is found that the shape of planar AEP do not change as the number of the MoS\(_2\) layers changes from 1 to 6. For a-Al\(_2\)O\(_3\) surface, the planar AEP in the atomic region has no obvious periodicity. The value of macroscopic AEP for MoS\(_2\) surface is -13.06 eV while its values is -18.31 eV for a-Al\(_2\)O\(_3\).

Figure 4 shows band alignment between a-Al\(_2\)O\(_3\) and MoS\(_2\). In the following, we discuss the VBO and CBO at a-Al\(_2\)O\(_3)/MoS\(_2\) interface in Fig. 04 based on HSE and GGA-PBE calculations. The VBO and CBO based on HSE calculations are 1.39 eV and 1.77 eV for 1-layer MoS\(_2\), 1.86 eV and 1.72 eV for 2-layer MoS\(_2\), and 1.76 eV and 1.94 eV for 3-layer MoS\(_2\). For 4-layer MoS\(_2\), the band gap is increased to 2.10 eV and 1.63 eV for 4-layer MoS\(_2\), and 2.07 eV and 1.74 eV for bulk MoS\(_2\). Previous investigations have indicated that VBO and CBO can be affected by the thickness of MoS\(_2\) layers.\(^{12}\) The VBO and CBO based on GGA-PBE calculations are 0.48 eV and 1.55 eV for 1-layer MoS\(_2\), 0.89 eV and 1.59 eV for 2-layer MoS\(_2\), 0.88 eV and 1.71 eV for 3-layer MoS\(_2\), 0.91 eV and 1.68 eV for 4-layer MoS\(_2\), and 1.00 eV and 1.69 eV for bulk MoS\(_2\). GGA-PBE underestimates the band gap, which leads to inaccurate VBO and CBO.\(^{15,25}\) The VBM and CBM positions of a-Al\(_2\)O\(_3\) and MoS\(_2\) are shown in Fig. 04. The VBM position of monolayer MoS\(_2\) is -5.94 eV for GGA-PBE, and -6.15 eV for HSE, which is close to previous results of -5.87 eV and -6.27 eV.\(^{15}\) It is noted that VBM position moves upward as the number of MoS\(_2\) layers is increased.

Figure 5 exhibits energy band diagrams for metal/a-Al\(_2\)O\(_3)/n-type MoS\(_2\) MOS under negative and positive voltages. The energy band near MoS\(_2\) will bend upwards as the negative voltage is applied between the metal and MoS\(_2\).\(^{69}\) The MoS\(_2\) surface layer changes from the majority carrier depletion to the minority carrier inversion with the increase of the voltage. In this case, the hole tunneling barrier of \(\phi_{HV, B}\) is determined by VBO. Leakage current is expressed as \(J_{HV, B}\). The energy band near MoS\(_2\) will bend down as the positive voltage is applied to devices. The MoS\(_2\) surface layer is in minority carrier accumulation region with the increase of the positive voltage. In this case, the electron tunneling barrier of \(\phi_{ECB}\) is determined by CBO. The leakage current is written as \(J_{ECB}\). Similar analysis is also suitable for metal/a-Al\(_2\)O\(_3)/p-type MoS\(_2\) MOS. In our model, the carrier tunneling current is closely related to the VBO and CBO. The band offset is sensitive to thickness of MoS\(_2\), which affects the leakage current of the device to a certain extent. At present, it is generally believed that VBO or CBO in ideal MOS device should be greater than 1 eV.\(^{24,25}\) It is noted that the VBO or CBO calculated by HSE for different MoS\(_2\) thickness is greater than 1 eV. Therefore, we believe that metal/a-Al\(_2\)O\(_3)/MoS\(_2\) MOS can be an ideal device.
FIG. 2. Band structures for bulk and different thickness layer of MoS$_2$. The blue and red point connections represent GGA-PBE and HSE results. The VBM is set to zero in order to check the band gap. The blue and red horizontal solid line in each panel indicates the CBM calculated by GGA-PBE and HSE functionals. The arrows indicate the band gap values. Special points in Brillouin zone are set as G (0 0 0); A (0 0 0.50); H (-0.33 0.67 0.50); K (-0.33 0.67 0); M (0 0.50 0); L (0 0.50 0.50).

**B. Impact of biaxial strain on the band alignment**

The biaxial strain of monolayer MoS$_2$ is defined as $\varepsilon = \frac{c-c_0}{c_0} \times 100\%$ where $c$ and $c_0$ are lattice constants of strained and non strained MoS$_2$, $\varepsilon > 0$ and $\varepsilon < 0$ corresponds to the tensile and compressive strain, respectively. Strain engineering may improve physical performances of semiconductors, in particular, their transport properties. This inspires us to study the effect of biaxial strain on monolayer MoS$_2$. The lattice strain is set in the range from -6% to 6% with the interval of 2%. Figure 6 presents the band structures for monolayer MoS$_2$ under biaxial strain. The monolayer MoS$_2$ is change to be a indirect band gap semiconductor under biaxial compressive strain, the VBM at K-point, and the CBM between K-point and G-point. The band gaps of GGA and HSE are increased to 1.83 eV and 2.38 eV for -2%, 1.69 eV and 2.26 eV for -4%, and 1.55 eV and 2.12 eV for -6%. The band gap first achieves the maximum value at $\varepsilon=-2\%$, and then gradually decreases with biaxial compressive strain. Similar results are also found on GaAs. The band structures of HSE are similar in shape with GGA-PBE, and the band gap values are increased by HSE functional. Interestingly, under biaxial tensile strain, the position of VBM shifts to G-point, and the CBM to K-point. The band gaps are decreased to 1.19 eV and 1.65 eV for 2%, 0.78 eV and 1.20 eV for 4%, 0.44 eV and 0.80 eV for 6%. It is noted that band gaps for monolayer MoS$_2$ will decrease with biaxial tensile strain, which is in agreement with previous investigation.

Figure 7 presents band alignment for a-Al$_2$O$_3$/monolayer MoS$_2$ interface under biaxial strain. The VBM and CBM position of a-Al$_2$O$_3$ and monolayer MoS$_2$ are shown in Fig. 7. The VBM of monolayer MoS$_2$ consists of $d_{x^2-y^2}$, $d_{xy}$ orbits of Mo and $p_x$, $p_y$ orbits of S. Its position originates from the repulsion between $d_{x^2-y^2}$, $d_{xy}$ orbits of Mo and $p_x$, $p_y$ orbits of S. The CBM of monolayer MoS$_2$ consists of $d_z^2$ orbit of Mo and $p_x$, $p_y$ orbits of S. Its position originates from the repulsion between $d_z^2$ orbit of Mo and $p_x$, $p_y$ orbits of S. This repulsion is closely related to the overlap of the d orbits of Mo and p or its of S, and their difference in energy. The overlap is gradually weakened as the biaxial strain changes from -6% to 6%. Therefore, the VBM and CBM of monolayer MoS$_2$ move downward as the strain changes from compressive strain to tensile strain. For GGA-PBE calculations, the VBO and CBO
are 1.00 and 1.12 eV for $\varepsilon=-6\%$, 0.58 and 1.38 eV for $\varepsilon=-4\%$, 0.50 and 1.33 eV for $\varepsilon=-2\%$, 0.42 and 2.05 eV for $\varepsilon=2\%$, 0.36 and 2.52 eV for $\varepsilon=4\%$, 0.28 and 2.95 eV for $\varepsilon=6\%$. For HSE calculations, the VBO and CBO are increased to 1.81 and 1.33 eV for $\varepsilon=-6\%$, 1.46 and 1.55 eV for $\varepsilon=-4\%$, 1.40 and 1.49 eV for $\varepsilon=-2\%$, 1.34 and 2.29 eV for $\varepsilon=2\%$, 1.27 and 2.80 eV for $\varepsilon=4\%$, 1.19 and 3.28 eV for $\varepsilon=6\%$. It is found from the results that the appropriate biaxial tensile strain in monolayer MoS$_2$ can increase the CBO, while the change of VBO is smaller, which effectively suppresses leakage current of the devices. Previously, Tabatabaei et al. have found that performance of MoS$_2$ field effect transistor can be improved significantly by biaxial strain, which is consistent with our investigation.

IV. CONCLUSIONS

The generation process of amorphous-Al$_2$O$_3$ sample is described by molecular dynamics and geometric optimization. The averaged bond lengths of O-O, Al-O and Al-Al for our amorphous-Al$_2$O$_3$ sample are agreement with previous simulations and experiments. The results show that our sample is close to the actual situation.

The band alignment of oxide and semiconductor can be obtained by building both surface and interface methods. We have verified the results by building SrTiO$_3$/TiO$_2$ interface. It is found that the surface and interface calculations can give similar results.

In order to avoid the waste of calculation time and
AEP distortion, we realize band alignment of amorphous-Al$_2$O$_3$/MoS$_2$ by building both amorphous-Al$_2$O$_3$ and MoS$_2$ surfaces. For HSE calculations, the VBO and CBO are 1.39 eV and 1.77 eV for 1-layer MoS$_2$, 1.86 eV and 1.72 eV for 2-layer MoS$_2$, 1.76 eV and 1.94 eV for 3-layer MoS$_2$, 2.10 eV and 1.63 eV for 4-layer MoS$_2$, and 2.07 eV and 1.74 eV for bulk MoS$_2$. The VBO and CBO can be changed by the thickness because the band gap of MoS$_2$ is sensitive to its thickness. The effect of VBO and CBO on the leakage current is also analyzed. 

The VBO and CBO based on HSE calculation are increased to 1.81 and 1.33 eV for $\varepsilon=-6\%$, 1.46 and 1.55 eV for $\varepsilon=-4\%$, 1.40 and 1.49 eV for $\varepsilon=-2\%$, 1.34 and 2.29 eV for $\varepsilon=2\%$, 1.27 and 2.80 eV for $\varepsilon=4\%$, 1.19 and 3.28 eV for $\varepsilon=6\%$. The positions of VBM and CBM for monolayer MoS$_2$ move downward as the strain changes from $\varepsilon=-6\%$ to $\varepsilon=6\%$. It is noted that the VBO and CBO are larger than 1 eV, indicating that metal/amorphous-Al$_2$O$_3$/MoS$_2$ is an ideal MOS device.

ACKNOWLEDGMENTS

The work is supported by the National Natural Science Foundation of China under Grant No. 11547182 and No. 11674037.

REFERENCES

1. G. E. Moore, Proceedings of the IEEE 86, 82 (1998).
2. G. He, X. Chen, and Z. Sun, Surface Science Reports 68, 68 (2013).
3. G. He, L. Zhu, Z. Sun, Q. Wan, and L. Zhang, Progress in Materials Science 56, 475 (2011).
4. Q. F. Fang, C. Hodson, M. Liu, Z. W. Fang, R. Potter, and R. Gunn, Physics Procedia 32, 379 (2012).
5. D.-G. Park, D. M. Diateuz, Z. Chen, S. N. Moham-mad, and H. Morkoç, Applied physics letters 69, 3025 (1996).
6. M. Hong, J. Kwo, A. Kortan, J. Mannaerts, and A. Sergent, Science 283, 1897 (1999).
7. F. C. Chiu, H. W. Chou, and J. Y. Lee, Journal of Applied Physics 97, 103503 (2005).
8. S. Wu, K. Chen, Y. Lin, C. Cheng, C. Hsu, J. Kwo, and M. Hong. Microelectronic Engineering 147, 310 (2015).
9. W. Cai, S. Stone, J. P. Pelz, L. F. Edge, and D. G. Schlam, Applied Physics Letters 91, 042901 (2007).
10. C. Hsieh, M. Chang, Y. Chien, L. Chou, L. Chen, and C. Chen, Nano Letters 8, 3288 (2008).
11. K. Xiong and J. Robertson, Microelectronic Engineering 86, 1672 (2009).
12. Y. Guo, L. Lin, and J. Robertson, Applied Physics Letters 102, 091606 (2013).
13. M. Choi, J. L. Lyons, A. Janotti, and C. G. V. De Walle, Applied Physics Letters 102, 142902 (2013).
14. B. Hoex, J. J. H. Gielis, M. C. M. V. De Sanden, and W. M. M. Kessels, Journal of Applied Physics 113, 113703 (2008).
15. F. Werner, B. Veith, D. Zielke, L. Kuhnemund, C. Tegenkamp, M. Seibt, R. Brendel, and J. Schmidt, Journal of Applied Physics 109, 113701 (2011).
16. L. Lin, Y. Guo, R. Gilten, and J. Robertson, Journal of Applied Physics 113, 134103 (2013).
17. D. Suh, D. Choi, and K. Weber, Journal of Applied Physics 114, 154107 (2013).
18. J. Liu, M. Y. Liao, M. Imura, H. Oosato, E. Watan-abe, A. Tanaka, H. Iwai, Y. Koide, and N. P. N. S. T. Ibaraki, Journal of Applied Physics 114, 084108 (2013).
19. C. Choi, E. Cartier, Y. Wang, V. Narayanan, and M. Khare, Microelectronic Engineering 84, 2217 (2007).
20. M. Olyaei, G. Malm, P. Hellstrom, and M. Ostling, Solid-state Electronics 78, 51 (2012).
FIG. 6. Band structures for monolayer MoS$_2$ under biaxial strain in the range from -6% to 6%. The bulk and red point connections represent GGA and HSE results. The VBM is set to zero in order to check the band gap. The blue and red horizontal solid line in each panel indicates the CBM calculated by GGA and HSE functional. The arrows indicate the band gap values. Special points in Brillouin zone are set as K (-0.33 0.67 0); G (0 0 0); M (0 0.50 0).

FIG. 7. Band alignment for a-Al$_2$O$_3$/monolayer MoS$_2$ interface under biaxial strain in the range from -6% to 6%. The VBM and CBM position of a-Al$_2$O$_3$ and monolayer MoS$_2$ are shown in Fig. Solid black lines represent the HSE results; Red and blue lines represent the GGA-PBE results.

21. J. X. Zheng, G. Ceder, T. Maxisch, W. K. Chim, and W. K. Choi, Physical Review B 75, 104112 (2007).
22. J. Kang, E. Lee, and K. J. Chang, Physical Review B 68, 054106 (2003).
23. K. Xiong, Y. Du, K. Y. Tse, and J. Robertson, Journal of Applied Physics 101, 024101 (2007).
24. A. Cota, B. P. Burton, P. Chan, E. Pavn, and M. D. Alba, Journal of Physical Chemistry C 117, 10013 (2013).
25. I. Costina and R. Franchy, Applied Physics Letters 78, 4139 (2001).
26. J. W. Liu, A. Kobayashi, J. Ohta, H. Fujioka, and M. Oshima, Applied Physics Letters 103, 172101 (2013).
27. B. Hu, M. Yao, R. Xiao, J. Chen, and X. Yao, Ceramics International 40, 14133 (2014).
28. E. A. Chagarov and A. C. Kummel, Ecs Transactions 16, 8 (2008).
29. G. Gutierrez and B. Johansson, Physical Review B 65, 104202 (2002).
30. P. Lamparter and R. Kniep, Physica B: Condensed Matter 234, 405 (1997).
31. K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, Y. Zhang, S. V. Dubonos, I. V. Grigorieva, and A. A.
Firsov, Science 306, 666 (2004).
32 C. V. Nguyen and N. N. Hieu, Chemical Physics 468, 9 (2016).
33 N. A. Lanzillo, T. P. ORegan, and S. K. Nayak, Computational Materials Science 112, 377 (2016).
34 J. Chang, Journal of Applied Physics 117, 214502 (2015).
35 J. Chang, L. F. Register, and S. K. Banerjee, Applied Physics Letters 103, 223509 (2013).
36 L. Banerjee, A. Mukhopadhyay, and A. Sengupta, Journal of Computational Electronics 15, 919 (2016).
37 K. Nishiguchi, A. Castellanos-Gomez, H. Yamaguchi, A. Fujiwara, H. S. J. V. D. Zant, and G. A. Steele, Applied Physics Letters 107, 053101 (2015).
38 J. Kang, S. Tongay, J. Zhou, J. Li, and J. Wu, Applied Physics Letters 102, 012111 (2013).
39 S. W. Han, H. Kwon, S. K. Kim, S. Ryu, W. S. Yun, D. H. Kim, J. H. Hwang, J. S. Kang, J. Baik, H. J. Shin, and S. C. Hong, Physical Review B 84, 045409 (2011).
40 S. Das, H. Y. Chen, A. V. Penumatcha, and J. Appenzeller, Nano Letters 13, 100 (2012).
41 A. K. Singh, R. G. Hennig, A. V. Davydov, and F. Tavazza, Applied Physics Letters 107, 053106 (2015).
42 S. Son, S. Yu, M. Choi, D. Kim, and C. Choi, Applied Physics Letters 106, 021601 (2015).
43 J. P. Perdew, K. Burke, and M. Ernzerhof, Physical review letters 77, 3865 (1996).
44 M. D. Segall, P. J. D. Lindan, M. Probert, C. J. Pickard, P. J. Hasnip, S. J. Clark, and M. C. Payne, Journal of Physics: Condensed Matter 14, 2717 (2002).
45 S. Lee, D. G. Cahill, and T. H. Allen, Physical Review B Condensed Matter 52, 253 (1995).
46 Y. Oka, T. Takahashi, K. Okada, and S. I. Iwai, Journal of Non-Crystalline Solids 30, 349 (1979).
47 J. Heyd, G. E. Scuseria, and M. Ernzerhof, The Journal of Chemical Physics 118, 8207 (2003).
48 J. Heyd and G. E. Scuseria, The Journal of chemical physics 121, 1187 (2004).
49 J. Paier, M. Marsman, K. Hummer, G. Kresse, I. Gerber, and J. Úgyvándy, Journal of Chemical Physics 125, 249901 (2006).
50 J. Heyd, J. E. Peralta, G. E. Scuseria, and R. L. Martin, The Journal of chemical physics 123, 174101 (2005).
51 J. L. Lyons, A. Janotti, and C. G. V. De Walle, Microelectronic Engineering 88, 1452 (2011).
52 C. G. V. De Walle, M. Choi, J. R. Weber, J. L. Lyons, and A. Janotti, Microelectronic Engineering 109, 211 (2013).
53 M. Choi, A. Janotti, and C. G. V. De Walle, Journal of Applied Physics 113, 044501 (2013).
54 J. W. Liu, A. Kobayashi, K. Ueno, J. Ohta, H. Fujioka, and M. Oshima, e-Journal of Surface Science and Nanotechnology 10, 165 (2012).
55 V. Afanasev, S. Shamuilia, A. Stesmans, A. Dimoulas, Y. Panayiotatos, A. Sotiropoulos, M. Houssa, and D. Brunco, Applied physics letters 88, 132111 (2006).
56 T. Windhorn, L. Cook, and G. Stillman, Electron Device Letters, IEEE 3, 18 (1982).
57 K. F. Mak, C. Lee, J. Hone, J. Shan, and T. F. Heinz, Physical Review Letters 105, 136805 (2010).
58 R. H. French, S. J. Glass, F. S. Oluchi, N. X. Xu, and W. Y. Ching, Physical Review B 49, 5133 (1994).
59 G. He, L. Zhu, M. Liu, Q. F. Fang, and L. D. Zhang, Applied Surface Science 253, 3413 (2007).
60 A. Ohta, M. Yamaoka, and S. Miyazaki, Microelectronic Engineering 72, 154 (2004).
61 L. Qiya, F. Zebo, J. Ting, L. Shiyani, T. Yongsheng, C. Jiajun, and Z. Yanyan, Chinese Physics Letters 31, 027702 (2014).
62 R. H. French, Journal of the American Ceramic Society 73, 477C489 (1990).
63 L. Silvestri, J. Cervenka, S. Prawer, and F. Ladouceur, Diamond and Related Materials 31, 25 (2013).
64 N. R. D’Amico, G. Cantele, and D. Ninno, Applied Physics Letters 101, 141606 (2012).
65 J. R. Weber, A. Janotti, and C. G. V. D. Walle, Journal of Applied Physics 109, 033715 (2011).
66 W. Liu, W. T. Zheng, and Q. Jiang, Physical Review B 75, 235322 (2007).
67 L.-B. Shi, X.-Y. Liu, and H.-K. Dong, Journal of Applied Physics 120, 105306 (2016).
68 Y. L. Yang, X. L. Fan, C. Liu, and R. X. Ran, Physica B 434, 7 (2014).
69 Y. C. Yeo, Q. Lu, W. C. Lee, T.-J. King, C. Hu, X. Wang, X. Guo, and T. Ma, Electron Device Letters, IEEE 21, 540 (2000).
70 P. Das, G. Dalapati, D. Chi, A. Biswas, and C. Maiti, Applied Surface Science 256, 2245 (2010).
71 C. Van de Walle, M. Choi, J. Weber, J. Lyons, and A. Janotti, Microelectronic Engineering 109, 211 (2013).
72 Q. Q. Sun, Y. Shi, L. Dong, H. Liu, S. J. Ding, and D. W. Zhang, Applied Physics Letters 92, 102908 (2008).
73 Q.-Q. Sun, C. Zhang, L. Dong, Y. Shi, S.-J. Ding, and D. W. Zhang, Journal of Applied Physics 103, 114102 (2008).
74 Q. Q. Sun, W. Chen, S. J. Ding, M. Xu, H. L. Lu, H. C. Lindhrengifo, D. W. Zhang, and L. K. Wang, Applied Physics Letters 90, 142904 (2007).
75 T. P. Kaloni, Y. Cheng, and U. Schwingenschlogl, Journal of Applied Physics 113, 104305 (2013).
76 L. Liu, X. Wu, X. Liu, and P. K. Chu, Applied Surface Science 356, 626 (2015).
77 S. Yu, H. D. Xiong, K. Eshun, H. Yuan, and Q. Li, Applied Surface Science 325, 27 (2015).
78 P. Chang, L. Liu, L. Zeng, and G. Du, Solid-State Electronics 113, 68 (2015).
79 Y. Zhang, M. Fischetti, B. Sorée, W. Magnus, M. Heyns, and M. Meuris, Journal of applied physics 106, 083704 (2009).
80 V. Fiori, S. Gallois-Garreignot, H. Jaouen, and C. Tavernier, Microelectronics Reliability 53, 229 (2013).
81 S.-Y. Cheng, M.-H. Lee, S. Chang, C.-Y. Lin, K.-T. Chen, and B.-F. Hsieh, Thin Solid Films 544, 487 (2013).
82 W.-T. Chern, P. Hashemi, J. T. Tehranl, D. A. Antoniadis, and J. L. Hoyt, Electron Device Letters, IEEE 35, 309 (2014).
83 L. B. Shi, M. B. Li, X. M. Xiu, X. Y. Liu, K. C. Zhang, C. R. Li, and H. K. Dong, Physica B 510, 13 (2017).
84 G. B. Liu, D. Xiao, Y. Yao, X. Xu, and W. Yao, Chemical Society Reviews 44, 2643 (2015).
85 S. Mohammad Tabatabaei, M. Noei, K. Khaliji, and M. Pourfath, Journal of Applied Physics 113, 163708 (2013).