Two-dimensional BaFCl monolayer: tunable bandgap and pronounced deep ultraviolet absorption

Zhenxue Zhu

College of Electronic and Optical Engineering, Nanjing University of Posts and Telecommunications, Nanjing, Jiangsu, 210023, China

*Corresponding author’s e-mail: 1125847214@qq.com

Abstract. Two dimensional (2D) wide bandgap materials have attracted a lot of attention due to their unique structural and optoelectronic properties. Based on the first principle calculations, we report a 2D wide bandgap BaFCl monolayer with an indirect bandgap of 5.58 eV. Remarkably, the bandgap can be flexibly tuned by applying external strain or electric field (E-field). Especially, monolayer BaFCl undergoes the transition from indirect bandgap semiconductor to direct bandgap semiconductor under small compressive strain, and a semiconductor-to-metal transition can be achieved by applying the electric field of 0.8 V/Å. In addition, monolayer BaFCl exhibits strong optical absorption in deep ultraviolet (UV) spectrum. These results render monolayer BaFCl as an attractive 2D material for application in flexible nanoelectronic and optoelectronic devices.

1. Introduction

The successful isolation of graphene by mechanical exfoliation [1] totally refreshes the people’s minds. From then on, 2D materials have become the research focus in several domains of science due to their unique structural and optoelectronic properties. These 2D materials, such as silicone [2], arsenene [3], and molybdenum disulfide (MoS2) [4], provide many attractive chances for industrial applications including lubrication, photovoltaics, hydrogen storage, and transistors. However, the bandgaps of most 2D pristine materials, especially monolayer materials, are lower than 3.40 eV, which apparently hinders their application in high temperature and high pressure environments [5]. This situation results in the extensive efforts in searching other 2D materials with wide bandgaps such as boron nitride (BN) [6], gallium oxide (Ga2O3) [7], and aluminium nitride (AlN) [8].

Wide bandgap semiconductors exhibit two specific merits for optical and electronic applications owing to their wide bandgap. The wide bandgap energy is more liable to absorb or emit UV light than narrow bandgap energy in optoelectronic devices [9]. Furthermore, a higher electric breakdown field can be provided by the wide bandgap energy, and thus the electronic devices can possess the higher breakdown voltages [9]. These advantages of wide bandgap semiconductors make them widely used in solid-state lighting, high power devices, and sensors. For example, SiC is a wide bandgap semiconductor, which has been used in field effect transistor, schottky diode, and current rectifiers [10].

It is well known that the higher electronegativity difference among the constituent atoms can induce the larger bandgap [11]. Halogens are more electronegative than other elements in the same row of the periodic table. Whether the combination of halogen elements and metallic elements can obtain a 2D intrinsic material with a wide bandgap? Excitingly, the layered bulk BaFCl with the wide bandgap has been synthesized in 1974 [12]. Furthermore, many layered materials have been
successfully exfoliated into monolayer structures using mechanical exfoliation or liquid phase exfoliation technique. For example, single layer MoS$_2$ and WSe$_2$ have been successfully prepared in experiment by the mechanical exfoliation approach [13]. This motivates us to explore whether there exists a stable monolayer BaFCl with a wide bandgap.

In this work, we systematically explore the stability, electronic and optical properties of the monolayer BaFCl based on the first principles calculations. The stability of monolayer BaFCl is assessed by various approaches. We find that monolayer BaFCl is an indirect semiconductor with a wide bandgap of 5.58 eV. Both the external strain and E-field are considered to tune the bandgap of monolayer BaFCl. Interestingly, monolayer BaFCl can maintain its indirect semiconducting property under strains except for the uniaxial compressive strain beyond 2% and the biaxial compressive strain beyond 4%, which could cause a transition from the indirect semiconductor to the direct one. The applied E-field can induce a semiconductor-to-metal transition in the system. In general, both the external tensile strains and E-fields can reduce the bandgap of monolayer BaFCl, while the bandgap first increases under a uniaxial compressive strain of 2% and then decreases with the further increased strain. Furthermore, monolayer BaFCl shows a pronounced deep UV absorption, suggesting its potential application in optoelectronic devices.

2. Computational details
We perform the calculations using density functional theory (DFT) [14], as implemented in the Cambridge Sequential Total Energy Package (CASTEP) [15]. The generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (PBE) functional is used for exchange-correlation functional [16]. The spin-orbit coupling (SOC) [17] is considered due to the existence of heavy element Cl atoms. To correct the PBE bandgaps, the Heyd-Scuseria-Ernzerhof (HSE06) screened hybrid functional with SOC effect is adopted [18]. The kinetic cutoff energy is set to be 600 eV for the plane-wave basis set, and a Monkhorst Pack k-point mesh of 12×12×1 is used for the geometry optimization and optoelectronic properties calculations. To avoid the interaction between two neighboring layers along the c-axis, a large vacuum space of 25 Å is used. Structural optimizations are stopped until the total energy, atomic force, and maximum stress are lower than 5×10$^{-7}$ eV/atom, 1×10$^{-2}$ eV/Å, and 2×10$^{-2}$ GPa, respectively. The phonon dispersion curve of the monolayer is calculated by linear response method.

3. Results and discussion
3.1. Structural and Electronic Properties of Monolayer BaFCl
Before investigating the electronic properties of monolayer BaFCl, we should explore the geometrical structure firstly. Bulk BaFCl crystallizes in PbFCl-type tetragonal structure and has P4/nmm space group [19]. The lattice parameters of primitive cell of optimized BaFCl are $a = b = 4.39$ Å, $c = 7.22$ Å (not shown). Each Ba atom bonds to four F and four Cl atoms, respectively. The corresponding bond lengths are 2.65 Å and 3.27 Å, respectively. Furthermore, bulk BaFCl is a semiconductor with a direct bandgap of 5.37 eV calculated by PBE+SOC method. As shown in figure 1a, both the valence band maximum (VBM) and the conduction band minimum (CBM) are located at Γ point.

We calculate the binding energy of monolayer BaFCl defined as 
$$\Delta E = E_{\text{monolayer}} / N_{\text{monolayer}} - E_{\text{bulk}} / N_{\text{bulk}},$$
where $E_{\text{monolayer}}$ and $E_{\text{bulk}}$ are the total energies of the monolayer BaFCl and the bulk BaFCl, and $N_{\text{monolayer}}$ and $N_{\text{bulk}}$ are the corresponding total atom numbers of the monolayer and bulk systems, respectively. Monolayer BaFCl has a formation energy of 97 meV, which is consistent with the weak electrostatic and vdW interactions. In addition, the formation energy of monolayer BaFCl is comparable to those of graphene, BN, and MoS$_2$ [20-21]. The results suggest that the common synthetic methods of 2D nanomaterials such as mechanical cleavage and liquid phase exfoliation methods can also be used to manufacture monolayer BaFCl.

Next, we build and optimize the monolayer BaFCl structure. As shown in figure 1b, the optimized BaFCl monolayer has a buckled rectangle structure with the thickness of 5.55 Å and consists of Cl-F-
Ba-F-Cl five sublayers. One unit cell of monolayer BaFCl consists of two Ba atoms, two F atoms, and two Cl atoms with the optimized lattice constants being $a = b = 4.29$ Å, which are smaller than that of bulk BaFCl. Each Ba atom forms four Ba-F bonds and Ba-Cl bonds. The lengths of Ba-F and Ba-Cl bonds are 2.63 and 3.25 Å, respectively. The length of Ba-F bond is smaller than that of Ba-Cl bond, indicating the stronger interaction between Ba and F atoms.

Figure 1. (a) The electronic band structure of bulk BaFCl based on PBE+SOC (b) Top and side views of the fully relaxed structure of monolayer BaFCl in a 4×4×1 supercell. The yellow dashed lines represents the primitive cell. (c) Phonon dispersion of monolayer BaFCl.

To investigate the stability of monolayer BaFCl, we assess its cohesive energy defined as $E_{coh} = \frac{(2E_{Ba} + 2E_{F} + 2E_{Cl} - E_{BaFCl})}{6}$, where $E_{Ba}$, $E_{F}$, $E_{Cl}$, and $E_{BaFCl}$ are the total energies of a single Ba atom, a single F atom, a single Cl atom and one unit cell of monolayer BaFCl, respectively. The monolayer BaFCl has a cohesive energy of 5.09 eV/atom, which is higher than those of monolayer AlP (4.10 eV/atom) [22], monolayer GeSe (4.37 eV/atom) [23], and silicene (3.71 eV/atom) [24], indicating that monolayer BaFCl is a strongly bonded network. We also consider the chemical stability of monolayer BaFCl. BaCl$_2$ and BaF$_2$ are selected as the reference compounds due to their stable structures. The reaction equation is BaCl$_2$ + BaF$_2$ → 2BaFCl, and the corresponding formation energy, calculated from formula $E_f = \frac{2 \times E_{BaFCl} - E_{BaCl_2} - E_{BaF_2}}{2 \times 3}$ (where $E_{BaFCl}$, $E_{BaCl_2}$, and $E_{BaF_2}$ are the total energies of monolayer BaFCl, BaCl$_2$, and BaF$_2$, respectively) is -0.038 eV/atom. It means that monolayer BaFCl can be thermodynamically stable with respect to phase separation into BaCl$_2$ and BaF$_2$. The phonon dispersion curves are calculated to evaluate the kinetic stability of monolayer BaFCl. As shown in figure 1c, no appreciable imaginary phonon modes can be found in the entire Brillouin zone, confirming the good kinetic stability of monolayer BaFCl.

After verifying the structural stability of monolayer BaFCl, we explore the electronic properties. Figure 2a shows the band structure calculated with PBE+SOC (HSE06+SOC) level of theory. The CBM is located at Γ point, while the VBM is located at X-M path, indicating that monolayer BaFCl is an indirect semiconductor. The bandgap of monolayer BaFCl is 5.58 eV (7.12 eV). It is larger than the values of GaN (3.4 eV) [25], diamond (5.5 eV) [26], and ZnS (3.7 eV) [27], demonstrating that the monolayer BaFCl is a wide bandgap semiconductor. That is to say, monolayer BaFCl is suitable for the application in high temperature and high pressure environments. Furthermore, the wide bandgap means that monolayer BaFCl based nanodevices can exhibit higher ON/OFF ratio and threshold voltage than those of narrow bandgap materials [28].

To further investigate the nature of the band structure, the projected density of states (PDOS) for monolayer BaFCl are exhibited in figure 2b. The hybridization of Ba-5d, F-2p and Cl-3p orbitals results in the formation of bonding states in valence bands region. The Ba-6s5d orbitals dominate the
electronic states near CBM coupled with small amount of F-2p and Cl-3p states. In addition, the character of Ba-F and Ba-Cl bonding can be evaluated based on the Hirshfeld charge and overlap population analysis. The transferred charges from Ba to F and Cl are 0.26 e and 0.18 e, respectively. Simultaneously, the calculated values of bond population for Ba-F and Ba-Cl are 0.12 and 0.41, respectively, revealing that monolayer BaFCl is combined by Ba-F and Ba-Cl ionic bonds.

Figure 2. (a) The electronic band structure of monolayer BaFCl under PBE+SOC and HSE06+SOC level. (b) The projected density of states of monolayer BaFCl under PBE+SOC level.

Figure 3. (a) Calculated bandgaps for monolayer BaFCl versus uniaxial strain along \(a\) or \(b\) direction. (b) The energies of states A and B as a function of uniaxial strain. The inset shows the location of states A and B in the valence band of strain-free structure.

3.2. Effect of External Strain on the Electronic Properties of Monolayer BaFCl

The tunable bandgap manipulation of 2D materials is important for their wider applications. It is reported that applying external strain is an effective approach to engineer the electronic properties of many nanomaterials. Herein, we explore the effect of external strain on the bandgap of monolayer BaFCl. The adopted external strain is defined as \(\varepsilon = (l - l_0) / l_0\), where \(l\) and \(l_0\) are the strained and the initial lattice parameters of monolayer BaFCl, respectively. The uniaxial and biaxial strains are applied in the range from -8% to 8% on the monolayer BaFCl. For uniaxial strain, we just analyze the variation of bandgap versus strain along \(a\) direction, because applying uniaxial strain along \(a\) and \(b\) direction generates the same adjustment of the bandgap.

The computations prove that the external strain has a rather pronounced effect on the bandgap of monolayer BaFCl. Figure 3a shows the curve of bandgap versus uniaxial strain along \(a\) or \(b\) direction (the band structures of monolayer BaFCl under uniaxial strain along \(a\) direction are shown in figure 4).
The bandgap of monolayer BaFCl decreases with increasing tensile strain. Specially, with increasing the tensile strain up to 8%, the bandgap decreases to 5.20 eV. When subjected to a compressive strain, the bandgap of monolayer BaFCl first increases to 5.59 eV under a uniaxial compressive strain of -2%. As the compressive strain increases from 2% to 8%, the bandgap decreases to 5.40 eV. It can be seen that the bandgap of monolayer BaFCl is more sensitive to the tensile than the compressive strain.

Figure 4. Band structure of the monolayer BaFCl at PBE+SOC level under different uniaxial strain along a direction.

Especially, we note that the uniaxial compressive strains can induce the indirect-to-direct bandgap transition. We then explore the nature of the indirect-to-direct transition. As shown in figure 4, with increasing the compressive strain, the CBM remains at the Γ point, while the VBM shifts its position. As the compressive strain reaches 4%, the VBM shifts from X-M path to Γ point. The migration of VBM is mainly due to the competition between two valence band-edge states (labelled as states A and B). As shown in figure 3b, in the strain range from 0 to -2%, the energy of state B is always higher than that of state A, and thus state B represents the VBM. As the compressive strain increases larger than 2%, state A exhibits a higher energy than state B, and becomes the new VBM at Γ point. Therefore, monolayer BaFCl undergoes a transition from indirect to direct bandgap semiconductor when the compressive strain larger than 2%.

We also explore the effects of biaxial strain on the bandgap of monolayer BaFCl. As shown in figure 5a, for the biaxial compressive strain, the bandgap of monolayer BaFCl from a value of 5.58 eV is increased up to the maximal value of 5.60 eV at -2% strain and then drops with further increased compressive strain. For the biaxial tensile strain, the bandgap decreases to 4.84 eV with increasing the strain up to 8%. Similar to the uniaxial compressive strain, the biaxial compressive can also induce an indirect-to-direct bandgap transition. As shown in figure 5b, the bandgap transition originates from the competition of the states A and B (mentioned above). When the biaxial compressive strain increases higher than 4%, state A shows a higher energy than state B, and it represents the VBM at Γ point. This causes the transition from indirect to direct bandgap. Therefore, applying external strain is an effective approach to tune the bandgap of monolayer BaFCl, which could result in a wider range of application.
3.3. Effect of electric field on the electronic properties of monolayer BaFCl
In order to deduce the potential application of the monolayer BaFCl, investigating whether its electronic properties could be tuned by applying E-field is also necessary. Furthermore, it has reported that applying E-field can effectively tune the electronic properties of 2D semiconductors [29]. Therefore, we next explore the electronic properties of monolayer BaFCl under the influence of the external E-field. The E-field ranging from -0.8 to 0.8 V/Å is applied perpendicularly to the monolayer BaFCl along c direction. Figure 5c plots the bandgap of monolayer BaFCl as a function of the external E-field. One can observe that both the applied positive and negative E-field can greatly reduce the bandgap. With increasing the positive and negative E-field up to 0.6 V/Å, the bandgap decreases to 0.01 eV and 0.11 eV, respectively. Especially, when the strength of the positive or negative E-field is larger than 0.6 V/Å, we find that monolayer BaFCl transforms from a semiconductor to a metal. In contrast to the external strain, the indirect-to-direct bandgap transition cannot be found when an E-field applied.
To understand the effect of external E-field on the electronic properties of BaFCl, we provide the band structures under different E-field (figure 6). When an external E-field is applied, the position of VBM at the X-M path is almost unchanged, while the CBM (Γ point) shifts close to the Fermi level with increasing the E-field, thus resulting the decrease of the bandgap. It indicates that the CBM is more sensitive to the external E-field than the VBM. When the strength of the E-field reaches 0.8 V/Å, the bandgap vanishes and the monolayer BaFCl turns into a metal. Therefore, it can be concluded that the bandgap of monolayer BaFCl can be effectively tuned by applying an E-field. Meanwhile, the intriguing semiconductor-to-metal transition suggests a potential approach using monolayer BaFCl for the design of novel optoelectronic, spintronic and thermoelectric devices.

3.4. Optical properties of monolayer BaFCl

Besides the strain-tunable bandgap, monolayer BaFCl also display an excellent optical property. Two electric vector polarizations of the in-plane (110) and out-of-plane (111) directions are considered. The optical property can be measured from the frequency-dependent dielectric function \( \varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega) \), from which absorption coefficient could be obtained. The absorption coefficient \( a(\omega) \) can be calculated using the equation:

\[
a(\omega) = \frac{\sqrt{2\omega}}{e} \left[ \frac{\varepsilon_2(\omega)^2}{\varepsilon_1(\omega)} + \varepsilon_2(\omega) \right]^{\frac{1}{2}}.
\]

Figure 7 shows the in-plane and out-of-plane optical absorption coefficients. It can be seen that the highest absorption coefficients can reach the order of 10^5 cm^-1, which are comparable to that of h-BN and AlN[30]. This reveals that monolayer BaFCl exhibit strong optical absorption. Although the spectra show a broad absorption band covering from 5.2 to 15.3 eV, the absorption efficiency is relatively weak. A relatively narrow absorption band ranges from 15.3 to 26.3 eV, which corresponds to the deep UV range of the solar spectrum, while the absorption efficiency is much stronger. Monolayer BaFCl shows strong absorption in the deep UV region, which could serve as a promising material for deep UV photodetectors.

![Figure 7. Calculated in-plane and out-of-plane optical absorption spectra of monolayer BaFCl at the PBE+SOC level.](image)

4. Conclusion

In summary, by means of DFT calculations, the structural, electronic, and optical properties of monolayer BaFCl have been systematically explored. The results indicate that monolayer BaFCl is semiconducting with an indirect wide bandgap and shows strong absorption in deep UV range. Its bandgap can be effectively tuned by external stain or E-field. Interestingly, an indirect-to-direct
transition can be induced by uniaxial or biaxial strain, and a semiconductor-to-metal transition in the monolayer BaFCl can be achieved by applying a positive or negative E-field of 0.8 V/Å. It promotes monolayer BaFCl as a promising candidate for optoelectronic applications. Considering the recent progress on manufacturing the nanomaterials, we believe that monolayer BaFCl could be realized in experiment. Furthermore, we hope our work would motivate more theoretical and experimental efforts on investigating the electronic and optical properties of 2D wide bandgap semiconductors.

Acknowledgments
This work was supported by the National Natural Science Foundation of China (Grant Nos. 61974068 and 11704198) and the Summit of the Six Top Talents Program of Jiangsu Province (Grant No. 2015-XCL-022).

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