Single Layer Bismuth Iodide: Computational Exploration of Structural, Electrical, Mechanical and Optical Properties

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Layered graphitic materials exhibit new intriguing electronic structure and the search for new types of two-dimensional (2D) monolayer is of importance for the fabrication of next generation miniature electronic and optoelectronic devices. By means of density functional theory (DFT) computations, we investigated in detail the structural, electronic, mechanical and optical properties of the single-layer bismuth iodide (BiI₃) nanosheet. Monolayer BiI₃ is dynamically stable as confirmed by the computed phonon spectrum. The cleavage energy (E_{cl}) and interlayer coupling strength of bulk BiI₃ are comparable to the experimental values of graphite, which indicates that the exfoliation of BiI₃ is highly feasible. The obtained stress-strain curve shows that the BiI₃ nanosheet is a brittle material with a breaking strain of 13%. The BiI₃ monolayer has an indirect band gap of 1.57 eV with spin orbit coupling (SOC), indicating its potential application for solar cells. Furthermore, the band gap of BiI₃ monolayer can be modulated by biaxial strain. Most interestingly, interfacing electrically active graphene with monolayer BiI₃ nanosheet leads to enhanced light absorption compared to that in pure monolayer BiI₃ nanosheet, highlighting its great potential applications in photonics and photovoltaic solar cells.

Since the discovery of graphene and its excellent electronic/mechanical properties¹⁻², tremendous research efforts have been focusing on searching new two-dimensional (2D) materials such as hexagonal boron nitride, transition metal dichalcogenides, and transition metal halides³⁻⁹. These 2D materials are bringing revolutions to numerous advanced applications due to their unique and fascinating physical and chemical properties. For example, monolayer MoS₂ can be used as transistors with room-temperature current on/off ratios of 10⁸. The advantages of 2D materials are so appealing that it is strongly desirable to explore a wide range of 2D materials, other than graphene, to satisfy different purposes. For example, 2D materials with a suitable band gap would meet the needs of field effect transistors or optoelectronic devices¹⁰⁻¹². More interestingly, a new family of 2D materials, i.e., van der Waals type hetero-structures, can be assembled in a designed manner, which has already proven successful for a number of electronic applications in the area of ultrathin and flexible devices¹³⁻¹⁷. Over the past decade, a number of experimental methods have been developed to exfoliate layered materials in order to produce monolayer nanosheets, such as liquid exfoliation that involves oxidation, ion intercalation/exchange, or surface passivation by solvents¹⁸⁻¹⁹.

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Some theoretical methods have been developed and employed to search new quasi-two-dimensional (Q2D) materials such as particle swarm optimization (PSO), “atom substitution” and “mechanical exfoliation”. PSO is generally used to locate the global minimum structure. Using PSO, Li et al. discovered a novel 2D inorganic material, namely Be₂C monolayer, in which each carbon atom binds to six Be atoms in an almost planar fashion, forming a quasi-planar hexa-coordinate carbon moiety; Tan et al. predicted that the BSi₃ silicene containing planar cyclic six-membered silicon rings (c-BSi₃) is the global minimum of BSi₃ monolayer. Additionally, atom substitution to the common layered structure is used to construct other new types of 2D materials. For instance, by atom substitution of the considered single layer structure, Arunima et al. examined the structure, stability, and electronic properties of 2D material in the family of group-IV mono-chalcogenides. “Mechanical exfoliation” is applied to obtain monolayer directly from their layered bulk structures. Zhao et al. predicted that the freestanding Ca₂N monolayer could be exfoliated from the bulk, and therefore obtaining 2D electron gas in free space without resorting to electron doping.

Up to now, a diverse range of intriguing properties in 2D materials have been revealed, highlighting the potential use for important applications in energy, photonics and nanoelectronics. However, the practical applications based on 2D materials are still very limited, because they suffer from serious bandgap hurdles, e.g. the lack of obvious gap in graphene and too large gap in boron nitride. Single-layer transition metal dichalcogenides such as MoS₂ possess an appropriate bandgap, but are strongly influenced by metal contacts, interface traps, charged impurities, dielectric environment, and structural defects. Therefore, the search for new types of 2D structures is of paramount importance for the fabrication of next generation nanodevices.

Bismuth tri-iodide (BiI₃) is a typical metal halide, the stacking in bulk counterpart is in ABC order with highly ionic Bi-I bond within the layers and weak van der Waals interaction between layers. It has been used for room temperature gamma-ray detection, primarily due to its intermediate band gap, high density, and high effective atomic number. The structural, electronic and optical properties of BiI₃ crystal have been reported both experimentally and theoretically. Podraza et al. demonstrated the strong spin-orbital coupling (SOC) effect in bulk BiI₃. Meanwhile, the BiI₃ thin films and plates have been synthesized by different approaches such as thermal evaporation, hot wall technique and physical vapour deposition. Exploring the BiI₃ nanostructures is beneficial to gain insights into the properties of BiI₃ at the atomic scale. So far, single-layer BiI₃ nanosheet has not been synthesized. Under this context, a systematic theoretical investigation on its structure, stability, electronic, mechanical and optical properties can not only enhance our understanding to their intrinsic characteristics, but also provide useful guidelines for the experimental synthesis of monolayer BiI₃ and facilitate their practical applications.

In this work, by means of density functional theory (DFT) computations, we first evaluate the stability of monolayer BiI₃ and the feasibility to exfoliate it from the bulk phase. Subsequently the electronic, mechanical and optical properties of monolayer BiI₃ nanosheets are investigated. We find that the SOC is significant and can reduce bandgap by around 1.0 eV in monolayer BiI₃ nanosheet. In addition, the band gap can be modulated with a biaxial strain. Most interestingly, forming a 2D van der Waals type heterostructure by interfacing electrically active graphene with single-layer BiI₃ nanosheet can significantly enhance the visible light response, i.e., shifting the absorption edge by 2 eV for a hybrid graphene/BiI₃ nanocomposite compared to that for a pure single BiI₃ nanosheet, which suggests its potential applications in optoelectronics and photovoltaics.

**Computational details**

All the calculations were performed employing the generalized gradient approximation in the Perdew-Burke-Ernzerhof form (GGA-PBE) and the projector augment wave method, as implemented in Viena **ab initio** simulation package (VASP). A dispersion correction of the total energy (DFT-D3 method)
was used to simulate the long-range van der Waals interaction. The plane-wave energy cutoff was set to 400 eV for geometry optimization and to 500 for static electronic structure and optical property calculations. To study 2D systems under the periodic boundary conditions, a vacuum layer with a thickness of at least 20 Å is inserted to avoid the interaction between periodic images. All the geometry structures were fully relaxed until energy and force were converged to 1E \(-11\) eV and 0.005 eV/Å, respectively. Unit cell of BiI\(_3\) (containing 8 atoms) with 5 × 5 × 1, 9 × 9 × 1 and 17 × 17 × 1 Monkhorst–Pack k-point sampling were used for BiI\(_3\) monolayer geometry optimization, static electronic structure and optical property calculations, respectively. Phonon dispersion analysis was performed using the Phonopy code\(^{59}\) interfaced with the density functional perturbation theory\(^{60}\) implemented in VASP. In phonon calculations, an increased plane wave energy cutoff of 500 eV and an 11 × 11 × 1 k-point sampling were employed, accompanying with more stringent convergence criteria.

The hybrid graphene/BiI\(_3\) nanocomposite was simulated using a 1 × 1 unit cell for BiI\(_3\) which matches well with the 3 × 3 supercell of graphene. The corresponding lattice mismatch is about 2%. In nanocomposite calculations, the k-point mesh used for geometry optimization and static calculation was 5 × 5 and 15 × 15, respectively.

The frequency-dependent dielectric matrix was calculated for the BiI\(_3\) nanosheet and for the hybrid graphene/BiI\(_3\) nanocomposite. The imaginary part is determined by a summation over empty states using the equation\(^{52}\):

\[
\varepsilon''_{\alpha\beta}(\omega) = \frac{4\pi^2}{\Omega} \lim_{q \to 0} \frac{1}{q^2} \sum_{c,v,k} 2\omega_k \delta(\varepsilon_{ck} - \varepsilon_{vk} - \omega) \times \langle \mu_{ck+e_{\alpha}} | \mu_{vk} \rangle \langle \mu_{ck+e_{\beta}} | \mu_{vk} \rangle^* 
\]

where the indices \(c\) and \(v\) represent conduction and valence band states, respectively. \(\mu_{ck}\) refers to the cell periodic part of the orbitals at the k-point. A large number of empty (conduction) band states are included for the summation in the equation.

Results and Discussion

Structure of bulk and monolayer BiI\(_3\). The stacking order in a bulk Bismuth tri-iodide (BiI\(_3\)) is ABC with highly ionic Bi-I bond within the layers and weak van der Waals interaction between layers as shown in Fig. 1(a). The interlayer distance is 3.38 Å in the bulk BiI\(_3\). For single layer BiI\(_3\) (Fig. 1(b,c)), bismuth atom planes are located between top and bottom iodide atomic planes, which forms the sequence I–Bi–I plane. The bond length between bismuth and iodine atom is about 3.1 Å, which is similar to that in the bulk BiI\(_3\). The charge density distribution, as shown in Fig. 1(d,e), present the ionic Bi-I bond character in the monolayer BiI\(_3\).

Stabilities and feasibility to realize in experiment. Before the detailed electronic structure investigations, we firstly examine the dynamic stability of monolayer BiI\(_3\) nanosheet by calculating its phonon band structure along the high symmetry line from M to Gama to K to M (Fig. 2(a)). Clearly, no imaginary frequency appears in the whole 2D reciprocal space, which confirms the dynamic stability of the BiI\(_3\) monolayer.

Subsequently, we evaluate the atom binding energy \(E_b\), which is defined as \(E_b = [2E(Bi) + 6E(I) - E(BiI_3)]/8\), where \(E(Bi), E(I),\) and \(E(BiI_3)\) are the total energies of bismuth atom, iodine atom, and BiI\(_3\) sheet, respectively. Based on this definition, systems with stronger binding strength have larger (positive) \(E_b\) values. The positive binding energy (2.69 eV per atom) indicates that BiI\(_3\) monolayer is stable.

We then check the possibility to obtain BiI\(_3\) monolayer via a mechanical exfoliation strategy. Thermodynamically, the exfoliation process should overcome a cleavage energy \(E_{cl}\), which is determined by the interlayer coupling strength\(^{53}\). We simulated the separation of a BiI\(_3\) monolayer from a neighbouring tri-layer (inset of Fig. 2(b)). The corresponding cleavage energy as a function of distance is shown in Fig. 2(b). The cleavage energy of BiI\(_3\) (0.43 J/m\(^2\)) is comparable to the experimentally estimated value of graphite (0.37 J/m\(^2\)).\(^{54}\) By performing a scan on the separation distance \(d\) of the fracture, we obtain the theoretical cleavage strength \(\sigma\), which is defined as the maximum derivative of \(E_b\) (Fig. 2(b))\(^{53}\). The calculated cleavage strength is about 2.8 GPa, which is similar to the value of graphite (2.10 GPa). Since graphene\(^{55}\) and many other materials\(^{56}\) can be exfoliated to obtain 2D atomic crystals, we expect that BiI\(_3\) is also able to be exfoliated by either Scotch tape or atomic force microscopy tip\(^{57}\). Notice that, although the exfoliation process discussed here can be routinely used in laboratory, an effective way to produce BiI\(_3\) monolayer samples in industry is still an interesting goal to pursue.

Electronic properties. With the optimized monolayer BiI\(_3\) and confirmed dynamic stability, we now turn to study the ground-state band structure and density of states (DOS) of BiI\(_3\) monolayer (as shown in Fig. 3).

For comparison, we first check the band structure of bulk BiI\(_3\). The obtained indirect band gap of bulk BiI\(_3\) is 1.5 eV with SOC, which is consistent with previous first-principles estimation of 1.55 eV and is also in good agreement with the experimentally-measured band gap of 1.67 eV by Podraza et al\(^{40}\).

Then, we investigate the electronic properties for the monolayer. Monolayer BiI\(_3\) nanosheet is found to be an indirect semiconductor with a bandgap of 2.54 eV without SOC, which is slightly larger than that in its bulk counterpart (2.50 eV without SOC). When SOC is included, the obtained indirect band
The band gap for BiI$_3$ monolayer is reduced to 1.57 eV. The band gap reduction by the PBE-SOC method is mainly attributed to the downward shift of the conducting band edge due to the SOC effect. As we can see from the DOS (right column in the Fig. 3), the valence band maximum (VBM) is mainly composed of I atom.
and the conduction band minimum (CBM) is dominated by the orbitals of Bi atom. Apparently, the SOC effect reduces the energy level in the conducting band for Bi atom. Therefore, the above results clearly indicate the existence of strong spin orbit effect in monolayer BiI₃, and the accurate band gap only can be obtained by considering SOC. Note that the band gap of monolayer BiI₃ (1.57 eV by PBE+SOC method) perfectly matches the ideal band gap value of solar cell materials (1.5 eV). Therefore, we expect that monolayer BiI₃ may possess an excellent performance in harvesting the visible light.

Mechanical properties and the control of electronic properties under mechanical strain. Knowledge of the mechanical properties of a material provides important information in the selection of suitable applications. A material must have the required properties to function adequately and must be durable enough for the expected product lifetime. Stress-strain curves are an extremely important graphical measure of a material’s mechanical properties, which provide a preliminary overview of geometrical change during loading testing. In our computations, the strain is added through the change of lattice parameters, the lattice constant $a$ of the strained phase is determined by the percentage strain $h$ ($a = a_0 (1 + h)$), where $a_0$ is the equilibrium lattice constants at 0% at strain. The $h$ values are from 0 to 14% with an interval of 0.8%. To eliminate the artificial effect of the out-of-plane thickness of the simulation box on the stress, we use the second Piola–Kirchhoff stress $\sigma$ to express the 2D forces per length with units of Nm⁻¹. The changes of force in various strains indicate the stress–strain relationship.

Figure 4(a) presents the calculated stress-strain curve of BiI₃ monolayer under a biaxial tensile strain. Apparently, the relationship between the stress and strain is linear. The ultimate and breaking strength are at the same point, indicating that the BiI₃ monolayer is a type of brittle material. The ideal strength for the fracture of the BiI₃ monolayer is around 13%.

It is known that strain has remarkable effects in tailoring electronic, optical and transport properties of 2D semiconductors. Experimentally, the external strain can be applied to 2D materials by various techniques, for example by the mismatch of lattice constant and thermal expansion between the substrate and the film. Kim et al. have shown the possibility of applying nearly 30% strain to graphene by the use of stretchable substrates $^{59}$. Therefore a full analysis of the strain effect on the band gap and electronic structure of single layer BiI₃ is highly desired.

Figure 4(b) shows the band gap as a function of the biaxial strain, in which the band gap has a downward trend with increasing tensile strain, regardless the SOC is considered or not. Note that the BiI₃ sheet breaks up at 13%, thus we only study the strain up to this breaking point. With SOC, the change trend of band gap under different strains is moderate, the band gap keeps at 1.57–1.6 eV when the strain...
is less than 6%, then gradually decreases to 1.5 eV at 13%. Without SOC, the gap slowly decreases from 2.54 eV at 0% to 2.45 eV at 5%, then sharply declines to 2.15 eV at 13%. The detailed band structures of BiI₃ under different strains are shown in Supporting Information Fig. S1.

Generally, the properties of 2D nanomaterials are dependent on the thickness. Therefore, we evaluated the effect of thickness on the structure and bandgap-strain relationship. In terms of structure parameters and energy (Table 1), the equilibrium lattice constants are gradually reduced from 7.64 Å in monolayer to 7.60 Å in bilayer and then to 7.59 Å in tri-layer. The binding energy per atom ($E_b$) increases from 2.69 eV of monolayer to 2.73 eV of bilayer then to 2.74 eV of tri-layer, which is consistent with favourable inter-layer binding energies. The lattice length and binding energy of tri-layer (the thickest layer we studied) are still slightly different with those (7.54 Å and 2.76 eV) of bulk. Considering the demanding computational costs for systems with large thickness, we only evaluated the band gap of strained few-layer BiI₃ sheets (2 and 3 layers) without SOC to examine the thickness effect. Our DFT computations showed that the band gaps of 2- and 3-layers decrease with the increase of strain (inserted figure in Fig. 4(b)), which is similar with that for monolayer BiI₃. This indicates the downward trend is irrelevant to the thickness and the interlayer interaction is indeed rather weak. Therefore, BiI₃ bulk crystals would be an ideal platform to probe 2D electronic property, circumventing the challenge of preparing large-area, single-crystal monolayers.

**Optical properties of BiI₃ nanosheet and the graphene/BiI₃ vdW hetero-structure.** The investigation of optical properties can effectively evaluate the performance of a material in light harvesting, which would therefore benefit our exploration of their potential applications in photovoltaics. In the following we calculate the imaginary part of the dielectric function $\varepsilon_2(\omega)$ of pure BiI₃ sheet with SOC and without SOC as shown in the Fig. 5(a). When considering SOC, the first peak of $\varepsilon_2(\omega)$ is in between 1.5 and 2.0 eV, which is in agreement with the value (1.57 eV) of the SOC band gap in Fig. 3(b). Similarly, the first peak from the calculation without SOC, located between 2.5 and 3.0 eV, is consistent with the uncorrected band gap shown in Fig. 3(a). The calculated imaginary part of the dielectric functions of BiI₃ monolayer with SOC shows a red shift about 1.0 eV of absorption edge compared to that without SOC, which indicates the strong effect of SOC to the optical properties of BiI₃ nanosheet.

Recent experiments have shown that a new family of 2D van der Waals type complex based on the combination of highly conductive graphene and optically active MoS₂ can generate photon-excite electron-hole pairs within the band gap of MoS₂, allowing to achieve enhanced photocurrent in visible light region⁶⁰,⁶¹. To explore this effect, we investigated the geometric structure and optical properties of graphene/BiI₃ vdW hetero-structure (G/BiI₃) without SOC effect because it is difficult to include SOC.
for the large system. For the hybrid structure, the graphene covered on BiI₃ monolayer (insert figure in Fig. 5(b)), has a binding energy of 0.023 eV per atom with an equilibrium interlayer spacing of about 3.67 Å. Therefore, interaction between graphene and the BiI₃ monolayer is very weak, a typical van der Waals interaction.

As shown in Fig. 5(b), the calculated imaginary part of the dielectric functions of hybrid G/BiI₃ displays an abrupt peak at 0.1 eV, which demonstrates the red shift of absorption edge is as large as 2.0 eV compared to that for the pristine BiI₃ nanosheet. The peak at 0.1 eV also indicates the remarkable enhanced abilities to absorb low-energy photons. Furthermore, the hybrid G/BiI₃ absorbs more photons in visible light region (1.5–3.0 eV) because of the higher ϵ(ω). Therefore, the hybrid G/BiI₃ nano-composite is expected to display enhanced photo-catalytic activities under sunlight irradiation.

Conclusions

In summary, we theoretically investigated the stability, electronic, mechanical and optical properties of BiI₃ nanosheet by means of DFT computations. BiI₃ monolayer is dynamically stable, and it is rather feasible to exfoliate the monolayer from the bulk. The BiI₃ nanosheet is a brittle material with a breaking strain of 13%. The SOC effect is important to compute the band structure of BiI₃ nanosheet, and the 1.57 eV band gap (with the inclusion of SOC) matches the ideal band gap value of solar cell materials. Moreover, the band gap of BiI₃ monolayer is strain controllable, and the BiI₃ films are insensitive to the thickness. Most interestingly, interfacing electrically active graphene with BiI₃ monolayer shows enhanced light absorption compared to that in the pristine monolayer BiI₃ nanosheet. All these unique and exception properties endow BiI₃ nanosheet and its composites great potentials for photonics and photovoltaic solar cells.

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**Author Contributions**
F. M. and A. D. conceived the idea. F.M., Y. J. and G. G. performed the calculations. F. M., M. Z., Y. G, A. B., Z. C. and A. D. contributed to the analysis of the results and to the writing of the manuscript.

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