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Can fluorine and chlorine functionalization stabilize the graphene like borophene?

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ABSTRACT

During the last couple of years, borophene, novel two-dimensional materials made from boron atoms have attracted remarkable attentions. As an exciting experimental achievement, most recently graphene like borophene has been realized (arXiv:1712.08770), which however suffers from dynamical instability because of its electron-deficiency. Nevertheless, as it was theoretically confirmed, hydrogenated graphene like borophene structures are stable which were surprisingly very recently experimentally synthesized. Halogenated graphene like borophene is also expected to form B − Halogen bonds and thus form energetically favorable structures. The effects of halogenations for varying levels of coverage (B_1X_1, B_2X_1 and B_4X_1; X is F and Cl) on the properties of graphene like borophene such as the geometric structures, thermal stability, mechanical response, electronic structure and optical properties are systematically investigated by the first-principles methods. The stability of these structures is tested by phonon spectrum analyses and ab initio molecular dynamics (AIMD) simulations. The investigation of mechanical properties demonstrates their high in-plane stiffness and outstanding stretchability as well. Notably, B_1F_1 and B_1Cl_1 were found to present direct band gaps of 2.15 and 2.47 eV, respectively, according to the HSE06 functional results, which can be further finely tuned by applying mechanical strains. In contrast, B_2F_1 and B_2Cl_1 have metallic character. The optical calculations illustrate that applying different tensile strains on these monolayers result in blue and red shift in optical spectra, suggesting that they are potentially promising for the applications in optoelectronics and nanoelectronics. Interestingly, the in-plane optical anisotropy of these novel 2D materials is highly desirable for the design of polarization-sensitive photodetectors.

1. Introduction

Since the successful isolation of graphene in 2004 [1], an immense amount of research has been conducted in the field of two dimensional (2D) materials due to their unanticipated and fascinating properties [2–5]. Although the family of two-dimensional (2D) materials are rich and very diverse, only a few members of this family are monoelemental, such as the silicene [6], germanene [7], stanene [8] phosphorene [9,10] and penta-graphene [11]. Except the graphene which can form different sp^3, sp^2 and sp bondings [12], aforementioned monoelemental 2D materials present buckled structures due to their limited flexibility for the various bond formations. Notably, boron, the neighbouring element of carbon at the boundary between metals and nonmetals in the periodic table, exhibits similar behaviour as that of the carbon and involves the ability for a diverse bond formations, and thus stay stable in various forms, from zero-dimensional to three-dimensional crystals [12–15].

Nevertheless, the experimental realizations of 2D boron sheets so called borophene, have been successfully achieved only recently. In this regard, borophene monolayers with various atomic configurations with buckled [16] and flat [17] structures have been synthesized using the epitaxy growth of boron atoms on the silver metallic surface. These exciting experimental reports on the fabrication of borophene nanomembranes, promoted numerous theoretical studies, which interestingly confirmed the outstanding performances of these novel 2D monoelemental materials for the hydrogen storage [18,19], high capacity rechargeable batteries [20–27] and superconducting, magnetic, electronic, and chemical nanodevices [28–32], with excellent mechanical and thermal stability characteristics [33–38]. The remarkable prospects for the application of 2D boron based 2D materials, plays as an exceptional motivation for the future experimental endeavors. Recently, experimental realization and characterization of hydrogenated graphene like borophene, so called borophene hydride sheets with an empirical formula of B_1H_1 was successfully achieved by the exfoliation and complete ion-exchange between protons and magnesium cations in magnesium diboride [39]. Our recent theoretical study [40] confirmed that 2D borophene hydride illustrates very attractive properties, including: high stiffness and thermal conductivity, light adsorption and strain tuneable band-gap semi-conducting electronic character. Very

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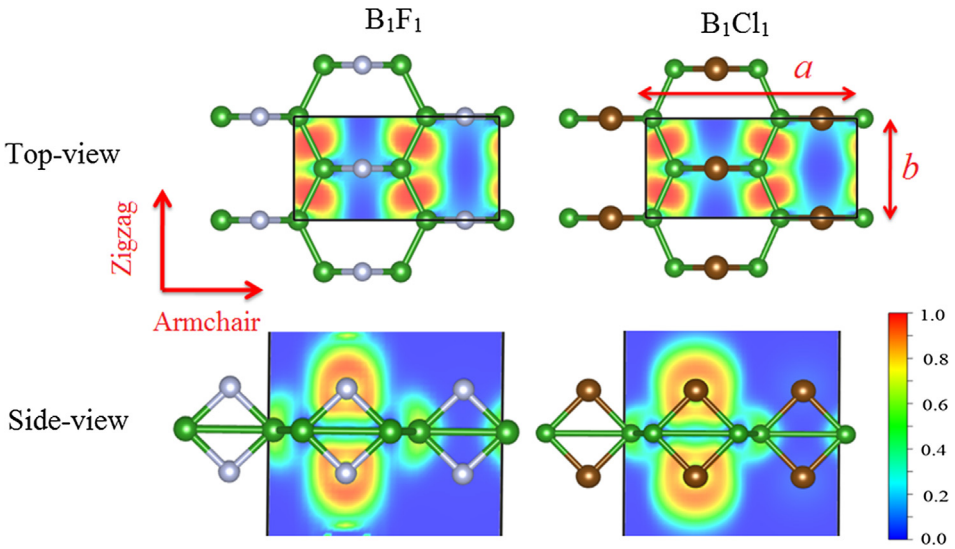

Fig. 1. The electron localization function together with top and side view of atomic configuration for single-layer B_1F_1 and B_1Cl_1 compounds. The black lines denote the B_4F_4 and B_4Cl_4 unit-cells which were used to evaluate mechanical, electronic and optical properties. The *a* and *b* lattice parameters of the unit-cells are also listed. Color code: boron (green), fluorine (light blue) and chlorine (brown). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 1
Summarized the lattice parameters, B—B bond lengths and B-halide bond lengths in Å for single layer B_1F_1, B_1Cl_1, B_2F_1 and B_2Cl_1.

Systems	*a*	*b*	B—B bond lengths without halogen bridging	B—B bond lengths with halogen bridging	B-halide bond length
B_1F_1	6.14	3.10	1.73	2.30	1.60
B_1Cl_1	6.81	3.20	1.75	2.69	2.01
B_2F_1	5.20	3.09	1.66	2.30	1.56
B_2Cl_1	4.80	3.14	1.67	2.07	1.95

recently, in an exciting experimental achievement [41] the pure graphene like borophene was for the first-time successfully synthesized on the aluminium surface using the molecular beam epitaxy technique under a ultrahigh vacuum condition. Nevertheless, due to the fact that boron has only three valence electrons, the electron deficiency makes the honeycomb lattice in the graphene-like borophene unstable [42]. The stability issues of this novel 2D structure can be eliminated by the hydrogenation, as it was experimentally [39] and theoretically [40,43] confirmed.

Based on experimental and theoretical works, the properties of other monoelemental 2D materials can be modified by covalent and

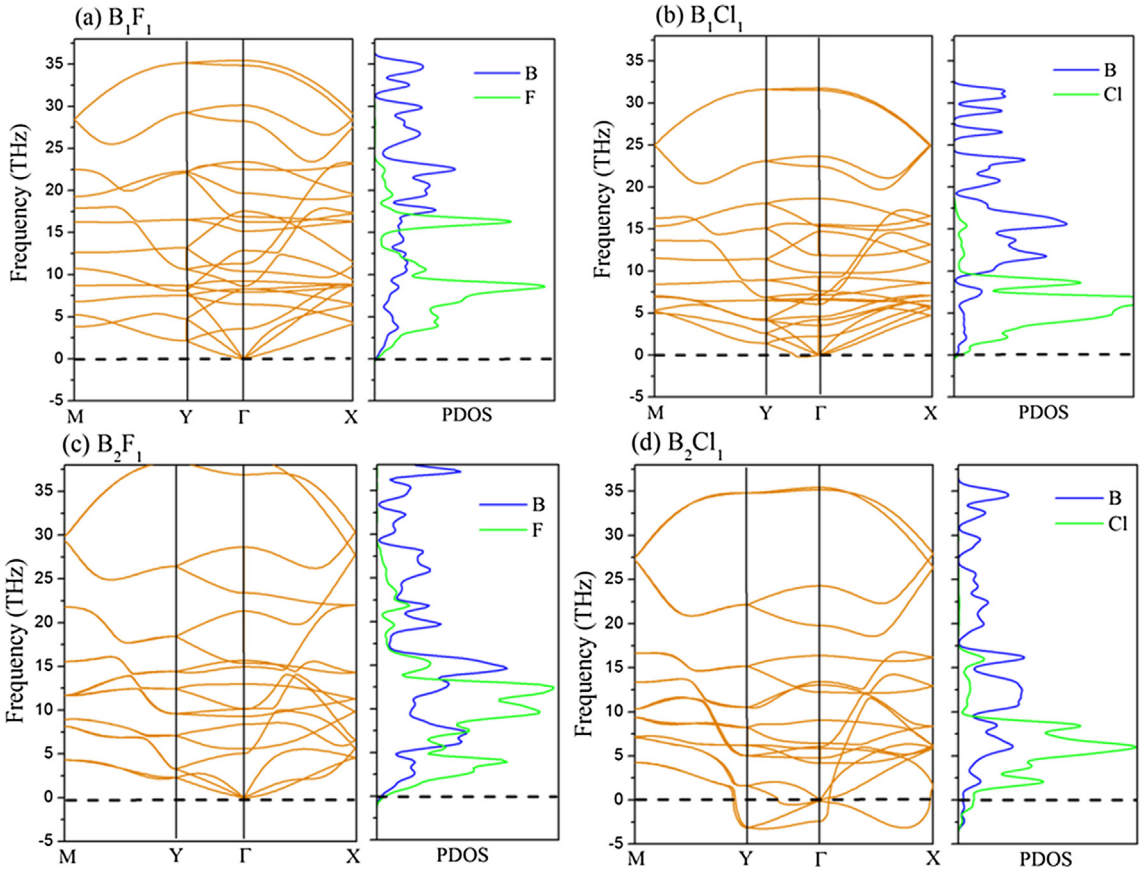

Fig. 2. Phonon dispersion and partial phonon density of states (PDOS) of single-layer (a) B_1F_1, (b) B_1Cl_1, (c) B_2F_1 and (d) B_2Cl_1.

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