Optik - International Journal for Light and Electron Optics 176 (2019) 579–585

Contents lists available at ScienceDirect

Optik

journal homepage: www.elsevier.com/locate/ijleo

Original research article

Beryllium chloride monolayer as a direct semiconductor with a tunable band gap: First principles study

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ARTICLE INFO

Keywords:
First principles prediction
BeCl monolayer
Electronic properties
Strain effect

ABSTRACT

By performing first principles calculations based on the density functional theory (DFT), a new two dimensional Beryllium chloride monolayer BeCl monolayer with a space group of 187-P6m2 is computationally predicted. It is found that the newly proposed BeCl monolayer indicates good stability suggests its great potential for experimental production. DFT based simulations reveal that the ground state of the predicted BeCl monolayer is a direct semiconductor moderate a wide band gaps can be modulated by mechanical effects. The results of this research show that BeCl monolayer has good potential applications in practical nano-electronic devices candidate especially in electro-mechanical sensors.

1. Introduction

In recent decade, inspired by the discovery of grapheme [1], two dimensional materials have attracted much attention due to their potential application in next generation of electronic and optical devices [2–9]. To find more practical applications, many theoretical as well as experimental studies have been done to find new two-dimensional monolayer materials [10–26].

Despite of many experimental limitations in producing two dimensional materials proposed by theoretical methods, when they compared to 3D materials, they exhibit many disadvantages limit restrict their practical applications. Therefore, it is needed to develop the production methods and to Improve the properties of 2D materials by predicting and designing new 2D materials.

In recent years, the experimental validations of theoretical predictions have attracted computational research groups to explore among the elements to find new stable two dimensional structures with novel physical properties. These studies have found many 2D materials. As examples, one can see group IV and group III-V two dimensional monolayer materials in honeycomb structure [27], monolayer group IV monochalcogenides (XY, X = S, Se, Te and Y = Si, Ge, Sn) which are semiconductors with wide band gaps [28–30], monolayer group III metal chalcogenides, MX (M = B, Ga, Al, or In and X = O, S, Se, or Te) such as InSe [31,32], GaS [33–35], GaSe [36,37], GaTe [38] that have been experimentally produced. Furthermore, in 2017, using first-principles simulations, the structural, mechanical, and electronic properties of group III-VI monolayers, MX (M: B, Al, Ga, In and X: Y = O, S, Se, Te) were investigated by Demirci et al. [39], where, the calculations show that the predicted MX monolayers are indirect band-gap semiconductors.

Inspired by the above mentioned MX monolayers, in the present work, a new stable two dimensional Beryllium Chloride monolayer compound is theoretically predicted and its possible electronic and optical properties are investigated. Our investigation is simply started by replacing M, X atoms in MX monolayer by Beryllium, and Chlorine atoms respectively. In our simulation, the first

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https://doi.org/10.1016/j.ijleo.2018.09.125
Received 21 July 2018; Accepted 23 September 2018

principles calculation in the frame work of the density functional theory (DFT) is used to lattice optimization, ground state stability checking, and the structural, electronic and optical properties calculation. In these calculations, Quantum Espresso code [40], and Wien2K [41] codes are employed. Investigating on its structural properties shows that the new proposed BeCl monolayer structures has good structural, kinetic, and thermal stabilities, thus it is a promising material to be realized. Also, analyzing its electronic and optical nature reveals that BeCl monolayer is a direct semiconductor with a tunable wide band gap. This paper is organized as follows:

The details of our theoretical study are presented in the next section. Section 3 presents the stability and the structural properties of the predicted BeCl monolayer. The electronic and optical characteristics of the designed 2D material are investigated in Section 4. Finally, the summary of our prediction is given in the last section.

2. Computational methods and details

The ground state of the proposed monolayer was obtained by joint atomic relaxation and cell lattice optimizations procedures by applieng density functional theory implemented in the QUANTUM ESPRESSO package. In these tasks the Martin-Troullier norm-conserving psedupotential [42] was considered for treating the core electrons while the energy cutoff was set to 60 rydberg for expanding the valance electrons wave functions. Moreover, the QUANTUM ESPRESSO package was also used in calculating phonon modes.

To calculate electronic and optical properties DFT based Wien2k code was employed. The electronic band structures as well as the density of states, were first calculated by the generalized gradient approximation (GGA) in the form of the Perdew-Burke-Ernzerhof exchange-correlation functional (PBE) [43], i.e., GGA-PBE level of theory. Also to get more accurate band gaps, the electronic band structures calculations were supported by future calculations based on Heyd-Scuseria-Ernzerhof (HSE06) hybrid functional theory [44]. In both calculations based on GGA-PBE, and HSE06 level of theories, the Kohn-Sham wave functions, were expanded by the full potential linear augmented plane waves plus local orbital (FPLAPW + lo), and k-point samples of $12 \times 12 \times 1$, and $22 \times 22 \times 1$ based on Monkhorst-Pack scheme [45] were used for electronic and optical properties calculations respectively. The computational input parameters of $R_{MT}K_{max} = 7$, $G_{max} = 14\ Ry^{1/2}$ and $l_{max} = 10$ were considered and a vacuum space of 15 Å in the non-periodic direction (z-axis) was utilized.

3. Optimized ground state properties

The initial model for BeCl monolayer was built according to the atomic configuration of abovementioned MX monolayers which some of them have been synthesized. Fig. 1 shows the atomic configuration of a possible stable BeCl monolayer. To find the optimized unit state of the BeCl monolayer, atomic coordinate and lattice parameters of the initially considered hexagonal atomic network were optimized simultaneously by using density functional theory implemented in quantum espresso package. In our optimization task a fully relaxed 2D structures belongs to the space group of 187-P6m2 with a lattice constant of 3.27 Å was obtained. The atomic configuration of the optimized unit cell of the BeCl monolayers from the top and the side views are presented in Fig. 1(a), (b). To find the accurate optimized lattice constant, by using Brich-Murnaghun thermodynamic equation state, the energy vs lattice parameter of

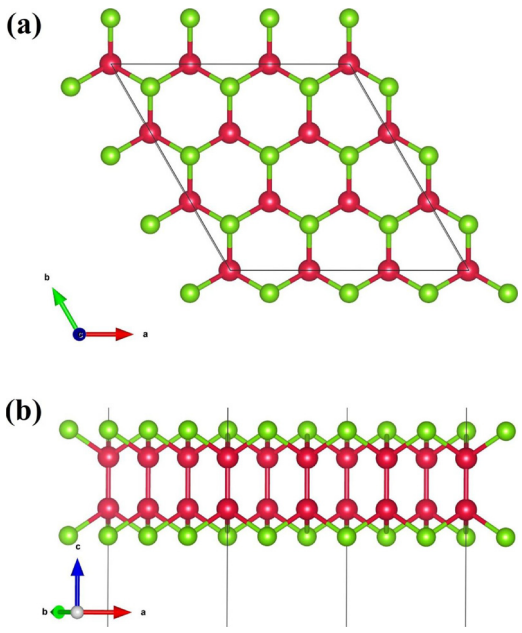

Fig. 1. Atomic structure of a 3 × 3 supercell of the predicted BeCl monolayers from the top (a) and the side views (b).