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Research Article

FORMATION OF NEW FORM OF GERMANENE ON *h*-BN SUBSTRATE

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ABSTRACT

Formation of the new germanene by deposition from the gaseous-like state onto the 2D hexagonal boron nitride substrate is studied via molecular dynamics simulations. This new form of germanene has a triangular honeycomb structure, and we call this new form 'triangular honeycomb germanene' (trh-germanene). The atomic structure of this trh-germanene is analyzed in detail by considering the coordination number and bond-angle distributions, ring statistics, interatomic distance distribution, buckling, and/or rippling of the sample. In addition, our density functional theory (DFT) calculations validate the existence of trh-germanene in both buckled and flat forms on the h-BN substrate, as well as in free-standing configurations. While the buckled trh-germanene exhibits greater stability than its flat counterpart, it remains less stable than conventional h-germanene.

Keywords: germanene with triangular honeycomb structure; MD simulation and DFT calculations; New form of germanene; Triangular honeycomb structure

1. Introduction

Germanene, a two-dimensional (2D) form of germanium with a buckled honeycomb structure, has been found and has been under intensive investigations by both experiments and computer simulations due to its potential applications (see Cai et al., 2013; Li et al., 2014; Matthes & Bechstedt, 2014). The objects of these studies are not only free-standing (and/or confined between two simple planar hard walls) germanene, but also germanene on various substrates. Good reviews about synthesis, atomic/electronic structure, or various phase transitions, as well as various behaviors and possible applications of germanene are

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highly recommended (Balendhran et al., 2015; Dimoulas, 2015; Kaloni et al., 2016; Ezawa et al., 2018; Bechstedt et al., 2021). Similarly, results of the simulations/calculations of various aspects of free-standing and/or confined germanene can be found (Malcolm & Nicol, 2016; Grassano et al., 2018; Nguyen et al., 2019). In addition, the stability, atomic and electronic structure of germanene on various substrates are discussed (Wang et al., 2016; Ni et al., 2017; Sante et al., 2019; Kubo, 2021). In particular, ab initio calculations of germanene on graphene-substrate show that graphene can serve as a good substrate for the synthesis of important 2D materials such as silicene or germanene (Cai et al., 2013). Weak substrate interactions have been found to favor the formation of low-buckled silicene or germanene and to preserve their linear band dispersion (Cai et al., 2013). Consistent with this, experiments have observed a buckled honeycomb germanene structure on Pt(111), and the atomic structure of the synthesized germanene has been characterized (Li et al., 2014) In addition, atomic/electronic structure as well as various behaviors of germanene formed on other substrates, including CdI_2-type 2D materials (Ni et al., 2017), Al(111) (Kubo et al., 2021) have also been studied. Moreover, combining ab initio calculations with a multi-orbital functional renormalization group analysis of Fermi surface instabilities in buckled germanene, it has been found that the interplay between monolayer and substrate coupling and the buckled honeycomb structure, provides a suitable scenario for unconventional triplet superconductivity (Sante et al., 2019).

Recently, experiments and DFT calculations have shown that germanene deposited on Al(111) adopts a kagome-like structure, rather than the honeycomb structure previously reported (see Kubo et al., 2021). Motivated by this finding, we investigate substrate-induced stabilization of alternative atomic configurations of germanene.

2. Calculations

It is important to adopt appropriate interatomic potentials for the system for which we carried out MD simulations, since the accuracy of the simulations depends strongly on the interatomic potentials. After checking carefully, the Tersoff interatomic potentials successfully used for BN-C nanostructures were taken for our *h*-BN substrate (Kinaci et al., 2012). In contrast, the Tersoff potential optimized for germanene was taken for interaction between Ge atoms (see Mahdizadeh & Akhlamadi, 2017). On the other hand, interactions between Ge atoms and B, N ones in the *h*-BN substrate were described by the Lennard-Jones potentials as done in a study by Mahdizadeh and Akhlamadi (2017). The same procedure of the deposition of C atoms from the gaseous state on the *h*-BN substrate was applied in the present work for the deposition of Ge atoms on the *h*-BN substrate (Nguyen et al., 2018).

Tersoff interatomic potentials have the form as follows:

$$V(ij) = f_c(ij)\left[a_{ij} f_R(r_{ij}) + b_{ij} f_A(r_{ij})\right] \tag{1}$$

$$f_R(r_{ij}) = A exp(-\lambda_1 r_{ij}) \tag{2}$$

$$f_A(r_{ij}) = B exp(-\lambda_2 r_{ij}) \tag{3}$$

where r_{ij} is the distance between atoms *i* and *j*, $f_R(r_{ij})$ is a pairwise repulsive term including orthogonalization energy when atomic wave functions overlap, and $f_A(r_{ij})$ is an attractive pairwise term which is related to bonding.

The initial model, including *h*-BN substrate, contains 15,000 atoms in total (5000 atoms for each type of atom: B, N, and Ge). A flat monolayer of perfect crystalline *h*-BN with the B-N bond-length of 1.45 Å served as a substrate, while 5000 Ge atoms were randomly distributed in the plane located at a distance of 5.01 Å above the substrate (Figure 1). The system was relaxed initially at 2,000 K for 2×10^5 MD steps to equilibrate. The initial temperature was adopted as high as 2000 K, and it was well above the melting point of crystalline germanene (T_m is ranged from 1,540 K to 1,670 K for defective and perfect germanene (Nguyen et al., 2020). The periodic boundary conditions (PBCs) are applied for the *x and y* directions, while the fixed boundary with an elastic reflection behavior is applied in the *z* direction. The relaxed system is cooling down from 2,000 K to 300 K at the cooling rates of 10^{11} and 10^{13} K/s using *NVT* ensemble simulations. The final models obtained at 300 K using the cooling rate of 10^{11} K/s were further relaxed for 10^6 MD steps before analyzing their structural characteristics. By contrast, the model obtained at 300 K with the cooling rate of 10^{13} K/s was relaxed for 10^5 MD steps to check the potential formation of an amorphous state.

Classical MD simulations were performed with a 1.0 fs time step. Temperature was controlled using simple velocity rescaling. We used LAMMPS software for MD simulations (Plimpton, 1995) and ISAACS software for calculating ring statistics (Le Roux & Petkov, 2010). We also used took VMD software for 2D visualization of atomic configurations (Humphrey et al., 1996). The cutoff radius of 2.80 Å for the Ge-Ge atomic pair was used to calculate coordination number and interatomic distance, and it was also applied in the ring statistics and bond-angle distribution calculation. This cutoff is equal to the first minimum following the first peak in the radial distribution function (RDF) of models at 300 K. Ring statistics were computed using the "shortest-path" criterion (Le Roux & Petkov, 2010). The initial h-BN substrate was constructed as a flat atomic sheet in the plan with $z=0$. After creating the simulation box, B and N atoms was allowed to move freely. However, due to the high thermal stability of the *h*-BN substrate, the substrate structure remained unchanged during the entire MD simulations. In contrast, Ge atoms were to move within the simulation box (Figure 1).

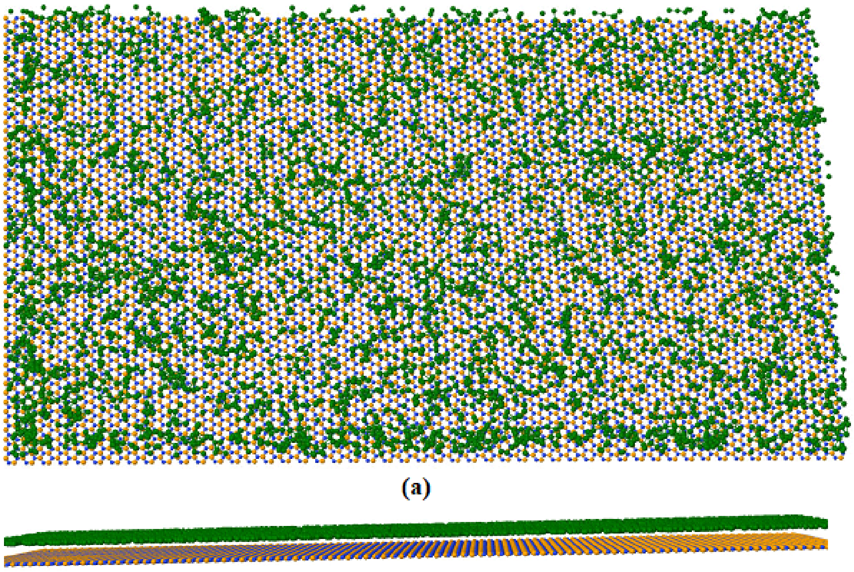

Figure 1. *3D visualization of atomic configuration with initial random distribution of Ge atoms above h-BN substrate*

3. Results and discussions

3.1. Formation of germanene from the gaseous-like state on h-BN substrate

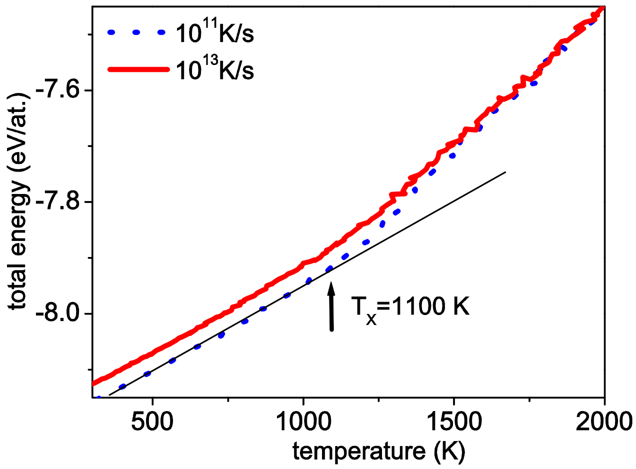

Figure 2. *Temperature dependence of the total energy of the system upon cooling from 2,000 K to 300 K at two cooling rates*

We now examine the formation of *trh*-germanene during cooling from the gaseous state of the state with initially random distribution of Ge atoms from 2,000 K to 300 K, mimicking the chemical vapor deposition of Ge atoms onto *h*-BN substrate. Figure 2 shows the temperature dependence of total energy of the Ge atomic configurations obtained upon cooling from 2,000 K to 300 K at two cooling rates (10^{11} and 10^{13} K/s).

Below a certain specific temperature, down to 300 K, the curve becomes linear, indicating that a rigid germanene has completely formed. For the cooling rate of 10^{11} K/s, this temperature is $T_X = 1100$ K, which is far below the melting point of germanene with the honeycomb structure (T_m ranging from 1,540 K to 1,670 K for defective and perfect germanene, respectively, Nguyen et al., 2020). It is noted that at the cooling rate of 10^{11} K/s, the formation of new 2D crystalline germanene with the triangular honeycomb structure was found (Figure 3). To detect the possibility of the formation of an amorphous state, the system was also cooled at a cooling rate as high as 10^{13} K/s. However, it leads to the formation of a crystalline state with a very large number of structural defects. We find that the diffraction pattern of this model consists of an ordered arrangement of bright points indicated the crystalline nature of the model (not shown). Because the amorphous state is beyond the scope of this work, we focus hereafter solely on the crystalline germanene formed at the cooling rate of 10^{11} K/s.

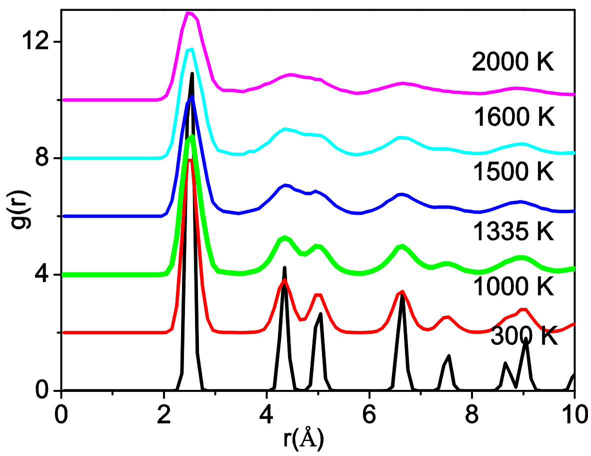

Figure 3. *Evolution of radial distribution function upon cooling from 2000 K to 300 K at a cooling rate of 10^{11} K/s*

Figure 3 shows the evolution of RDF of the germanene upon cooling from 2,000 K to 300 K. At 2,000 K, RDF exhibits gaseous-like behavior since it was rather smooth, and the first peak in RDF is not high (Figure 3). Upon further cooling, the peaks in RDF become more pronounced. By 1,000 K (i.e. at $T < T_X$, $T_X = 1100$ K, see Figure 2), many separated peaks in RDF occur. The peak intensities increase as the temperature decreases, as illustrated by the RDF at 300 K. This means that rigid 2D state has fully formed in the system (Figure 3). The first peak in RDF is located at around 2.50 Å, and this distance can be considered as the mean bond-length of the model.

More details of the evolution of the structure of the system upon cooling can be seen in Figure 4. Although 3-fold rings dominate in the system for the whole temperature range studied, ring distributions at relatively high temperature ($T > T_X$) remain broad, indicating a non-crystalline state of the model. In contrast, below $T_X = 1100$ K, the network comprises only three- and four-membered rings, with the three-membered rings accounting for 0.99 of the total at $T = 1000$ K (Figure 4d). This means that at temperatures below $T_X = 1100$ K, a rigid 2D crystalline state has completely formed as discussed above. Indeed, the well-relaxed atomic configuration obtained at 300 K exhibits a triangular honeycomb crystalline 2D structure (Figure 5). The diffraction pattern of the model consists of the ordered arrangement of bright points indicated a crystalline structure of the model (not shown). This is a new allotrope of 2D germanene which has not been reported in literature yet.

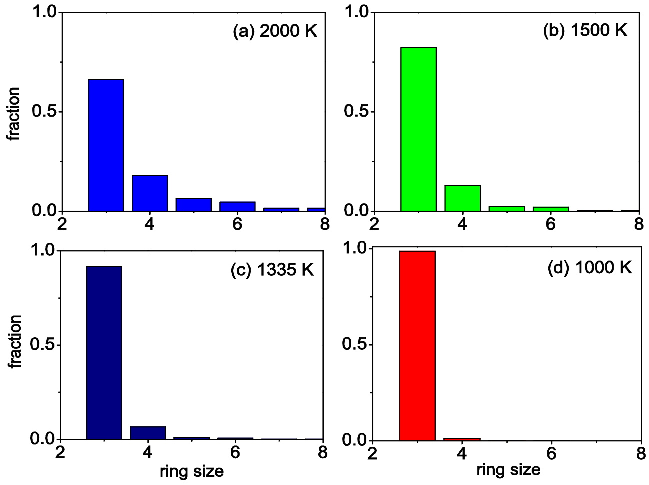

Figure 4. *Evolution of ring distribution upon cooling from 2000 K to 300 K at the cooling rate of 10^{11} K/s.*

3.2. Atomic structure of the triangular honeycomb germanene obtained at 300 K

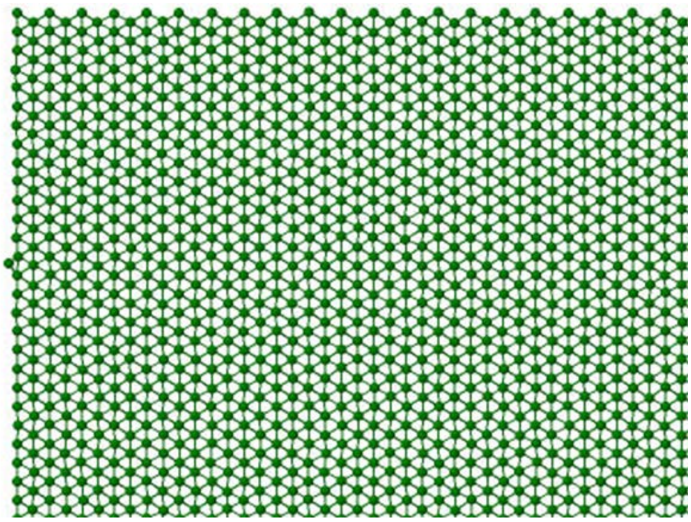

Figure 5*. 2D visualization of the enlarged left corner part of the atomic configuration of Ge atoms on h-BN substrate after relaxation at 300 K. The upper bound is the free edge, the right and lower boundaries are just cut from the large model, while the left boundary is under PBCs. We show only the configuration of Ge atoms, without the h-BN substrate*

Given the lack of prior reports on the microstructure of this newly identified 2D allotrope, it is therefore of interest to perform a detailed microstructural analysis of the trh-germanene obtained at 300 K in the present work. It is clear that *trh*-germanene obtained in the present work exhibits a nearly perfect 2D crystalline triangular honeycomb structure, i.e., the basic structural units of the material are triangles (Figures 5 and 6). There is a very small number of structural defects found in our model. We find only some mono-vacancies (Figure 6a) and 'adatoms' (Figure 6b). The adatom located above the triangle leads to the formation of a 3D tetragon (Figure 6b). Although the fraction of defects in *trh*-germanene is small, these defects can play an important role in physico-chemical performance of the material. More details of the microstructure of *trh*-germanene can be seen in Figures 7 and 8. First, most atoms in the model have a coordination number Z = 6 (Figure 7a). The fraction of atoms with Z = 6 is rather high equaled to 0.94. It is a specific coordination number of the triangular honeycomb 2D structure, and it may be related to the sp^3d^2 bonding in the *trh*-germanene. Existence of atoms with Z = 3, 4, and 5 can also be seen in Figure 7a. However, their fraction is very small. The local configurations around atoms with Z = 3, 4, and 5 can be considered as structural defects. These defects are mostly located in the edge region of the model (Figure 5).

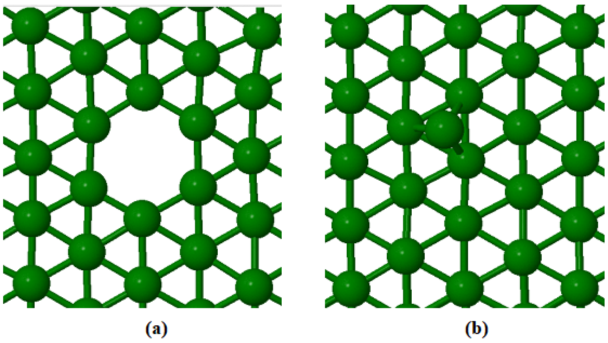

Figure 6. *Some specific defects in the trh-germanene obtained at 300 K: (a) Mono-vacancy; (b) 'Adatom'*

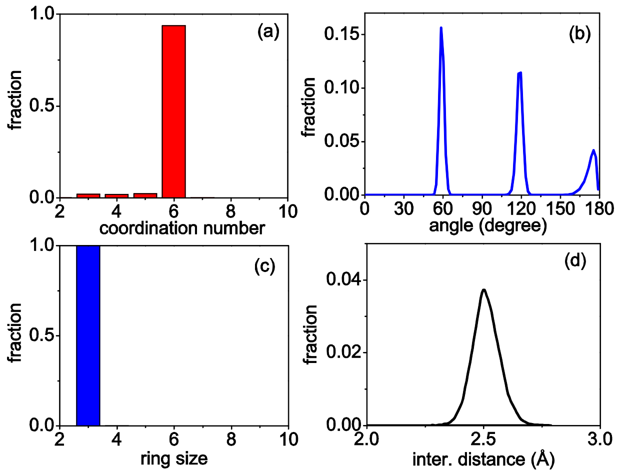

Figure 7. *Structural characteristics of the trh-germanene obtained at 300 K*

Because the flat *h*-BN substrate is much larger than the newly formed germanene sheet, i.e., the former contains 15000 atoms while the latter contains only 5000 atoms, the outermost Ge atoms along the *y* direction do not reach the periodic boundaries used in this work. In other words, the free edge of the Ge monolayer in the *y* direction is formed (see the upper boundary of the atomic configuration presented in Figure 5). This means that the Ge monolayer formed in the present work is a nanoribbon, rather than an infinite sheet.

Therefore, some defects can occur in the free edge region of the model. The bond-angle distribution of the Ge monolayer is also calculated, which has three narrow peaks (Figure 7b). The sharpest one is located at 58.50 °, which is close to the value of 60^o of the perfect triangular honeycomb 2D lattice. The second lower peak is located at 119.30^o, which is related to the angle inside the hexagons of the honeycomb structure. This peak is related mostly to the free edge of the Ge monolayer (Figure 5) or angles inside mono-vacancy (Figure 6a). For a perfect flat honeycomb structure, this angle should be equal to 120^o. The last peak is located around 175.50^o with very small fraction (Figure 7b). This peak is related to specific nearly linear local atomic configurations in the edge region (Figure 5). The next important characteristic is the ring distribution, and we find that fraction of 3-fold rings is of 0.999 (Figure 7c). The next structural behavior is an interatomic distance distribution which is narrow (ranged from around 2.34 Å to 2.69 Å, see Figure 7d). It has a sharp peak at around 2.50 Å. The value of 2.50 Å can be considered as the mean interatomic distance or the mean Ge-Ge bond-length of *trh*-germanene which is also equal to the position of the first peak in RDF of the model obtained at 300 K (Figure 3). The distribution of interatomic distance and mean interatomic distance found in the *trh*-germanene are comparable with those found for the germanene with honeycomb structure (Nguyen et al., 2019; Moreira et al., 2004). For the latter, it is found by MD simulations that the interatomic distance ranges from 2.29 Å to 2.66 Å, and the bond length is 2.45 Å (Nguyen et al., 2019). In contrast, DFT data gives the range from 2.33 Å to 2.44 Å (Moreira et al., 2004). Note that the Ge-Ge bond-length in 3D germanium is found to be 2.45 Å (Nguyen et al., 2019).

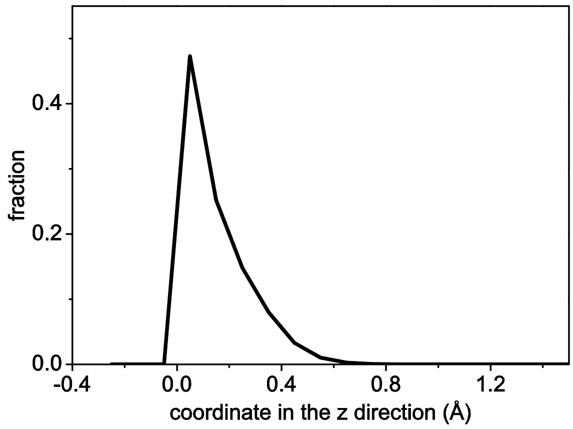

Figure 8. *Distribution of atomic coordinates in the z direction of the trh-germanene obtained at 300 K*

The last important structural behavior of *trh*-germanene is the distribution of atomic coordinates in the *z* direction of the *trh*-germanene obtained at 300 K, since it is related to the buckling/rippling of 2D materials. It is found that silicene and germanene have the buckled 2D structure, unlike the flat one of graphene. It is found by DFT calculations that the stable germanene with honeycomb structure has the buckling $\Delta z = 0.74$ Å (Nguyen et al., 2019). The buckling has a crucial role in many interesting behaviors of germanene (Nijamudheen et al., 2015). In particular, it leads to the occurrence of a direct band gap in hydrogenated germanene, and it also leads to the enhancement of the chemical reactivity of germanene with hydrogen to form germanene (Nijamudheen et al., 2015). Therefore, it is of great interest to study the possibility of the existence of buckling in *trh*-germanene. The flat *h*-BN substrate was located at $z = 0$ during the whole MD simulations, and the *trh*-germanene formed at 300 K upon deposition on *h*-BN was then relaxed for 10^6 MD steps prior to the structural analysis. In addition, the distribution of atomic coordinates in the *z* direction of the *trh*-germanene at 300 K is shown in Figure 8. One can see that the obtained *trh*-germanene is not flat. Some points can be drawn here:

- The deviation of the position of Ge atoms in the z direction ranges from around $z = 0.05$ Å to $z = 0.65$ Å. Most Ge atoms have $z = 0.05$ Å (the peak in the distribution is located at $z = 0.05$ Å, and their fraction is 0.47, see Figure 8) which is very close to the main plane of the *h*-BN substrate (i.e., it is located at $z = 0$ Å).
- The maximum deviation of Ge atoms from the main plane of *h*-BN substrate (at $z = 0$) is around 0.65 Å, which is smaller than the buckling of germanene with a honeycomb structure, and it is around 0.74 Å. Difference in the atomic structure, including that of the "buckling," may lead to quite different physico-chemical behaviors which would be explored by both MD simulations and ab initio calculations, and it is going on.

Note that various 2D materials with the triangular lattice structure have been found and studied. Recently, a 2D FeC compound with a triangle lattice structure was found by MD simulations (Vo, 2020). However, it is not a 2D triangular honeycomb structure, i.e., it should be a 2D triangular square lattice structure (Vo & Nguyen, 2019). In addition, the square-triangle lattice structure phase transition in a simple 2D system is found and discussed by MD simulations (Vo & Nguyen, 2019). This phase transition occurs in a martensitic manner; the new phase resulting from this phase transition is a triangular honeycomb structure 2D solid (Vo & Nguyen, 2019). Note that the triangular lattice 2D structure exists as a result of the square-triangle lattice phase transition in various systems such as flux line and vortex lattices, superconductors, Wigner crystals, skymion lattices, quantum Hall systems, colloids, diblock polymers, and the like (Vo & Nguyen, 2019).

4. Conclusions

We carried out intensive MD simulations of the chemical vapor deposition-like growth of free Ge atoms onto 2D *h*-BN substrate and found the formation of a quite new allotrope of germanene, i.e., *trh*-germanene, which has a triangular honeycomb lattice structure. The obtained *trh*-germanene has nearly perfect structure with a small amount of defects. The mean Ge-Ge bond length in the model is 2.50 Å, which is close to that of the germanene with the honeycomb structure. The atomic sheet of this new allotrope of germanene is not flat. In addition, our MD simulations confirm that due to high thermal stability, 2D *h*-BN can serve as a good substrate for the synthesis of various 2D materials, including their new allotropes. Our DFT optimization reveals the existence of free-standing *trh*-germanene, along with *trh*-germanene on the *h*-BN substrate. We found that *trh*-germanene exhibits metallic and non-magnetic behaviors.

❖ ***Conflict of Interest:*** *Authors have no conflict of interest to declare.*

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SỰ HÌNH THÀNH DẠNG MỚI CỦA GERMANENE TRÊN MÀNG ĐƠN LỚP h-BN

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TÓM TẮT

Sự hình thành germanene bằng cách lắng đọng từ trạng thái khí lên chất nền là boron nitride được nghiên cứu thông qua mô phỏng bằng phương pháp động lực học phân tử. Dạng germanene mới này có cấu trúc dạng tổ ong tam giác và chúng tôi gọi dạng mới này là 'gernamene tổ ong - tam giác'. Cấu trúc nguyên tử của trh-germanene này được phân tích chi tiết thông qua tính toán số phối vị và phân bố góc liên kết, thống kê vòng, phân bố khoảng cách giữa các nguyên tử, độ nhấp nhô của mô hình. Ngoài ra, các tính toán lý thuyết bằng DFT của chúng tôi xác nhận sự tồn tại của trh-germanene ở cả dạng nhấp nhô và dạng phẳng trên chất nền h-BN, cũng như trong các cấu hình đơn lớp. Trong khi trh-germanene nhấp nhô thể hiện độ ổn định cao hơn so với dạng phẳng tương ứng, thì nó vẫn kém ổn định hơn h-germanene thông thường.

Từ khóa: Germanene có cấu trúc tổ ong tam giác; mô phỏng MD và tính toán DFT; dạng mới của germanene; cấu trúc tổ ong tam giác