Physics Letters A 380 (2016) 768–772

Contents lists available at ScienceDirect

Physics Letters A

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A theoretical study on the electronic property of a new two-dimensional material molybdenum dinitride

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ARTICLE INFO

Article history:
Received 9 October 2015
Received in revised form 8 December 2015
Accepted 14 December 2015
Available online 18 December 2015
Communicated by R. Wu

Keywords:
Monolayered MoN_2
Electronic structure

ABSTRACT

Motivated by the recent synthesis of bulk MoN_2 which exhibits the layered structure just like the bulk MoS_2, the monolayered MoN_2 exfoliated from the bulk counterpart is investigated systematically by using density-functional calculations in this work. The result shows that the ground-state two-dimensional monolayered MoN_2 behaves as an indirect band gap semiconductor with the energy gap of ~0.12 eV. Subsequently, the external strain from −6% to 6% is employed to engineer the band structure, and the energy gap can be efficiently tuned from 0 to 0.70 eV. Notably, when the strain is beyond 5% or −3%, the two-dimensional monolayered MoN_2 would transfer from an indirect band gap to a direct band gap semiconductor. This work introduces a new member of two-dimensional transition-metal family, which is important for industry applications, especially for the utilization in the long-wavelength infrared field.
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1. Introduction

With the development of industry and the demand of smaller device and component, now it is transferring from microelectronic and nanoelectronic to atomic scale era. Consequently, the low-dimensional materials almost have been the most highlighted materials because they can just satisfy the above demand. As the representative of two-dimensional (2D) materials, graphene was discovered by Novoselov et al. early in 2004 [1,2]. Since then, the great interest of research was pumped into graphene and its analogues due to their unique properties and potential applications in electronics, optoelectronics, spintronics, catalysis, and so on [3–9]. Unfortunately, graphene has the characteristic of zero-gap and chemically inert, this prevents its utilization in some fields, such as transistor. Furthermore, some experimental explorations apparently confirmed that it was not possible to thermodynamically stabilize a single layer of atoms unless they were coupled to a bulk substrate [10–12], except graphene. This makes the graphene analogues must be generated on the substrate. However, owing to the interaction between the compound and substrate, the property of the freestanding compound would usually be changed when it is generated on the substrate.

The above fact motivates the researchers to explore other suitable 2D materials, and the monolayered transition-metal dichalcogenides (TMDs) with the general chemical formula MX_2 (M = Mo, W, Pt, X = S, Se, Te) have attracted great attention [13–19]. Although the layered TMDs are originated from the bulk one due to the weak interaction between layers in the corresponding bulk counterparts [20–22], the properties are very different, just like graphite and graphene. For instance, the 2D monolayered MoS_2 could transfer from an indirect band gap in bulk one to a direct band gap [23–25]. Particularly, the energy gap of some semiconducting 2D TMDs can be efficiently tuned by changing the external environment or the internal chemical environment, such as composition, thickness, strain, and so on. For instance, the band gaps of the most heavily studied 2D TMDs (MX_2, M = Mo, W, X = S, Se, Te) ranges from around 1.0 to 1.9 eV via tuning the chemical compositions, layer numbers, and external strains [14,25–29]. This attractive property of TMDs offers opportunities for potential applications in a variety of corresponding fields, including catalysis, energy storage, field-effect transistors, logic circuits, etc.

Nevertheless, an important electromagnetic wavelength range, the long-wavelength infrared regime starting at ~8 μm, still cannot be effectively shaded by the above 2D materials. This particular wavelength range is very important for some technological fields, such as range finding using LIDAR systems. Therefore, in order to design the smaller devices and systems applied in this distinct electromagnetic wavelength range, it is crucial for us to search for suitable 2D semiconducting materials covering this wavelength range.

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http://dx.doi.org/10.1016/j.physleta.2015.12.017
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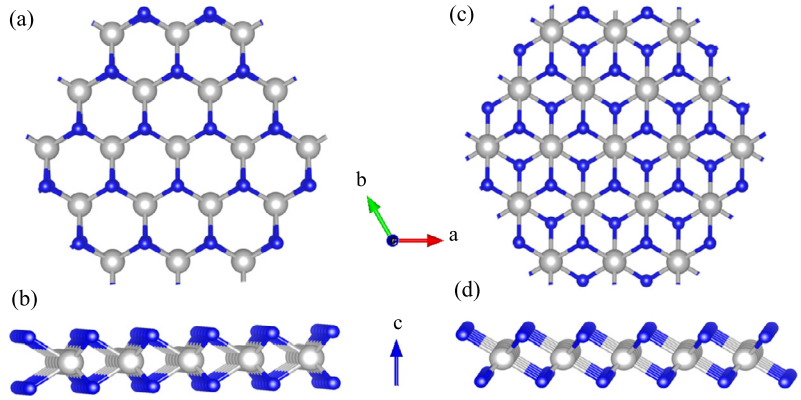

Fig. 1. (Color online.) (a) Top view for the 2D monolayered MoN_2 with H type structure (H–MoN_2), (b) side view for the H–MoN_2, (c) top view for the 2D monolayered MoN_2 with T type structure (T–MoN_2), (d) side view for the T–MoN_2.

Just recently, Wang et al. synthesized a new molybdenum dinitride MoN_2. Notably, MoN_2 possesses a rhombohedral $R3m$ structure, the very one isotypic with MoS_2. This tells that the monolayered MoN_2 is very likely to be exfoliated from the bulk counterpart, just like the obtainment of MoS_2 and other 2D TMDs. This fact motivates us to explore the property of 2D monolayered MoN_2 by using density-functional calculations. The result shows that the ground-state 2D monolayered MoN_2 exhibits the nature of an indirect band gap semiconductor. Subsequently, the strain is employed and efficiently engineers the 2D monolayered MoN_2 from an indirect band gap to a direct band gap semiconductor, with the band gap ranged from ∼0.12 to ∼0.70 eV. This work introduces a new member of 2D transition-metal family and gives an opportunity to search for other 2D monolayered transition-metal dinitride, which is significant for applications in modern industry.

2. Computational methods

In this work, the underlying *ab initio* structural relaxations and electronic band structure calculations were carried out by using generalized-gradient approximation (GGA) framework and the projector-augmented-wave (PAW) potentials as implemented in VASP [30,31]. The structural relaxations were performed until the Hellmann–Feynman force on each atom reduces by less than 0.001 eV/Å. To ensure high accuracy, the k-point density and the plane waves cutoff energy are increased until the change of the total energy was less than 10^{-5} eV, and the Brillouin-zone (BZ) integration is carried out using $14 \times 14 \times 1$ Monkhorst-Pack grid in the first BZ, the plane waves with the kinetic energy up to 600 eV is employed. In addition, the simulations were performed using a 2×2 supercell based on MoN_2 unit cell, and the repeated layered geometry is with a thick vacuum region of 25 Å.

3. Results and discussion

Firstly, the structural property of the 2D monolayered MoN_2 is investigated in detail. It is well known that the layered TMD crystals have two hexagonal lattices of MX_2 sandwiches, usually named H-TMD (the coordination is trigonal prismatic) and T-TMD (the coordination is octahedral) structures, respectively [20]. For this reason, although the experimentally synthesized bulk MoN_2 is stacked with monolayered H–MoN_2, the two types H–MoN_2 and T–MoN_2 structures are employed here, as pictured in Fig. 1. The result shows that the total energy of T–MoN_2 is about 0.29 eV per formula unit lower than that of H–MoN_2, telling that the ground-state structure of the exfoliated 2D monolayered MoN_2 would exhibit T type. This fact is different with the above mentioned molybdenum chalcogenide whose stable structures are H type. The structural stability of the predicted 2D monolayered T–MoN_2 is confirmed by the formation energy. The formation energy is defined as $\Delta E = E_{MoN_2} - E_{Mo} - E_{N_2}$, where E_{MoN_2} is the total energy of 2D monolayered T–MoN_2, and E_{Mo} and E_{N_2} are the total energies of crystal Mo and cubic gauche (cg) nitrogen, respectively. Thus the structure is thermodynamic stable or metastable when ΔE is negative. The result shows that ΔE is ~ -1.87 eV, indicating that the structure of 2D monolayered T–MoN_2 is stable. The length of Mo–N bond is ∼2.03 Å, and the distance between the two N layers is ∼2.17 Å. The lattice constant is ∼2.97 Å.

Next, the electronic properties of T–MoN_2 are systematically investigated. Fig. 2 plots the total density of states (DOS), partial density of states (PDOS), and band structure of T–MoN_2. Fig. 2(a) shows that T–MoN_2 has the semiconducting nature with an energy gap of ∼0.12 eV, and the Fermi energy level (E_F) is located at the valence band maximum (VBM). The PDOS of Mo and N ions indicates that the valence band is mainly composed of N $2p$ states and the conduction band is mainly composed of Mo $3d$ states. The band structure, as plotted in Fig. 2(b), tells that T–MoN_2 behaves as an indirect band gap semiconductor, because the conduction band minimum (CBM) and VBM are located at Γ and near M points, respectively, instead of the same reciprocal lattice point.

Applying strain has been an efficient method to engineer the properties of material, for instance, the strain can tune the electronic band gap and arouse the direct-to-indirect band gap transition of TMDs [32,33]. Here, both the compressive and tensile biaxial strains are employed to engineer the electronic structure of 2D monolayered T–MoN_2, and the strain is defined as $(a_T - a_{am})/a_{am}$, where a_{am} is the lattice constant of the structure at ambient condition, and a_T is the one under strain. Additionally, the strain is applied along a and b directions, as pictured in Fig. 3(a). The energy gap dependence on the strain is plotted in Fig. 3(b). It is clear that the energy gap can be efficiently tuned by small strain. Under the tensile strain, the energy gap decreases from 0.12 to 0 eV with increasing the strain up to 2%, indicating a semiconductor–metal transition. Next, a sudden increase of the energy gap from 0 to 0.70 eV appears when the strain increases up to around 3%, and subsequently the energy gap decreases from 0.70 to 0.50 eV with increasing the strain further. When the 2D monolayered T–MoN_2 is under the compressive strain, the energy gap increases from 0.12 to 0.32 eV with increasing the strain up to −3%, and then it decreases with increasing the strain further, and finally it becomes zero when the strain reaches around −6%, indicating that there is a semiconductor–metal transition at the compressive strain of around −6%. These results tell that the energy gap of T–MoN_2 could be efficiently tuned from 0 to 0.70 eV by applying small external strain.

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