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Electronic structure study on 2D hydrogenated Icosagens nitride nanosheets

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ABSTRACT

Metal nitride nanosheets has attracted remarkable importance in surface catalysis due to its characteristic ionic nature. In this paper, using density functional theory, we investigate geometric stability and electronic properties of hydrogenated Icosagen nitride nanosheets. Binding energy of the sheets reveals hydrogenation is providing more stability. Band structure of the hydrogenated sheets is found to be n-type semiconductor. Partial density of states shows metals (B, Al, Ga and In) and its hydrogens dominating in the Fermi region. Mulliken charge analysis indications that hydrogenated nanosheets are partially hydridic surface nature except boron nitride.

1. Introduction

Nanosheets become a most important materials after the discovery of graphene. Graphene, a 2D extended honeycomb network of sp2 hybridized carbon compound has attracted much attention in nanoscience [1,2] due to their possible applications in many emerging fields such as electronic devices [3], gas sensors [4], transparent conductors [5] and biological applications [6]. The impressive advancement in graphene research has inspired scientists to explore the properties of several 2D planar materials [7,8]. These 2D nanosheets are now considered to be an excellent candidates for

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future electronic applications such as high-Tc superconductors [9], optical [10], semiconductor [11] and magnetic superlattices [12].

Recently, researchers have also extended the 2D inorganic nanosheets, such as metals (Si [13], Ge [14]), metal oxides (ZnO [15], MgO [16] TiO2 [17]), metal nitrides (BN [18–20], AlN [21,22], GaN [23,24]), and metal disulfides (MoS2 [25], WS2 [26]) are the major interest to experimental as well as theoretical chemists [27,28]. Among these, Icosagens nitride (Group III-nitrides) nanosheets have been referred to be a potential equivalent of graphene owing to its various reasons like analogous lattice parameters, more resistant to oxidation, chemical and thermal stability [29,30]. Hydrogenation on nanosheets, is a current pursuit due to many of its remarkable properties it also known to decreases the internal stress, it alters the electronic, optical and magnetic properties.

In addition BN [31–34], AlN [35,36], and GaN [37,38], a binary compounds are experimentally synthesized in single and multiple layers and are widely used in semiconductor devices, however, only a few reports on fully hydrogenated sheets such as C [39–41], Si [41–43], Ge [41] BN [44–46], and AlN [47] are studied and other sheets are very limited, no periodic trends have been reported. So, it is worth looking into the possibility of fully hydrogenated group III nitride nanosheets, as in the same spirit as graphane and silicane [48].

In this paper, we report the density functional theory calculations to study the structural and electronic properties of fully hydrogenated Icosagens nitride (Ha–MN–Hb; M = B, Al, Ga and In) nanosheets.

2. Computational methods

The structural optimizations and electronic calculations were performed using Accelrys package with CASTEP code [49], which is based on density functional theory (DFT) and plane-wave pseudo potential method. The local density approximation (LDA) [50] form was adopted in the calculations. The cutoff energy for the plane wave basis was set to be 400 eV. All geometry optimizations and electronic structure calculations such as band structure, density of states and Mulliken charge population were performed using periodic boundary conditions, and Brillouin zone integrations are performed using a $7 \times 7 \times 1$ Monkhorst–Pack (MP) [51]. MP grids were also used for the calculation of the density of states (DOS). The criterion of convergence for the residual forces is set to be less than 0.01 eV/Å and the change of total energy less than 5×10^{-6} eV. The interlayer distance is set to more than 10 Å to avoid the interaction between the layers.

3. Result and discussion

3.1. Structure

The hydrogenated group III-nitride nanosheets are found to be similar structural lattice of graphane. In that, Nitrogen atoms and group III atoms are arranged in a honeycomb network of sp^3 hybridized 2D layers [8]. Fig. 1 represents the optimized structure of H_a–MN–H_b (M = B, Al, Ga and In) single layer nanosheets, which resembles pristine graphane sheet where each M and N atom is bonded to one N and M atoms respectively. In all the layers both M and N atoms are passivized by hydrogen in the polar surface H_a–M and H_b–N with bond lengths of 1.204–1.717 Å and 1.048–1.036 Å, respectively from

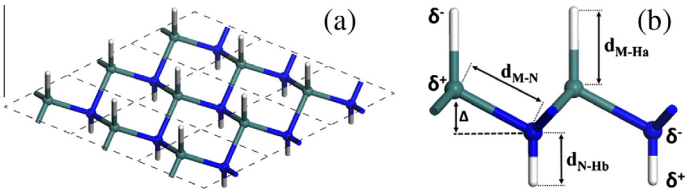

Fig. 1. (a) Optimized structure and (b) side view of 2D Ha–MN–Hb (M = B, Al, Ga and In) nanosheet.