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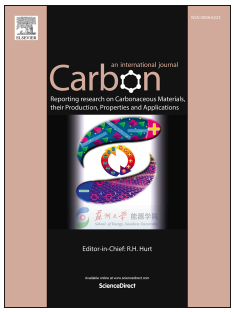


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# Structural characteristics and strain behaviors of two-dimensional $C_3N$ : First principles calculations

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**Abstract**

In this study, structural characteristics and strain behaviors of $C_3N$ are investigated by first principles calculations. First, we investigate the stacking behaviors of $C_3N$, and find the most stable order. Then, the band structure of $C_3N$ is investigated. We attempt to explain the disagreements between theoretical and experimental band gaps by impurity phase and biaxial strain. The band alignment at $\alpha-Al_2O_3/C_3N$ interface is presented. The valence band offset (VBO) and conduction band offset (CBO) are larger than 1.49 eV, which suggest that the interface is a promising candidate used on short channel transistors. Finally, the strain behavior of $C_3N$ is studied. It is found that the monolayer $C_3N$ at 273 K can withstand up to a strain level of $\varepsilon$=12% for zigzag and armchair uniaxial strain, and $\varepsilon$=10% for *ab* biaxial strain. The band edge position, effective mass and band gap under the strain are presented. The CBO increases with the strain, which suggests that appropriate tensile strain can effectively prevent the leakage current of the device. Our investigation can provide valuable information for insight into the novel $C_3N$ materials.

*Keywords:* Two-dimensional semiconductor, $C_3N$, Band alignment, Strain

## 1. Introduction

In recent years, the size of the transistor has entered the 10 nm regime. As the size of the transistor is reduced, the short channel effect is very significant [1–6]. In order to overcome this short channel effect, the high permittivity materials (high-k) have to be used to replace the traditional silicon dioxide [7, 8]. In addition, we have to replace the traditional semiconductor Si with two-dimensional (2D) semiconductor. 2D materials with few atomic layer thickness have attracted intense attentions since graphene's discovery [9–13]. 2D semiconductor has become an ideal candidate for the short channel devices due to smooth surface. However, graphene is greatly limited in the application of electronic devices because of its zero band gap problem [14]. In order to use graphene better, opening its band gap has become a key issue. It is generally believed that the band gap of graphene can be opened by changing the internal structure .

Theoretical and experimental studies have shown that nitrogen doped graphene may exhibit semiconducting properties, which have attracted attention [15–17]. Previously, graphitic carbon nitride ($g-C_3N_4$) nanosheets attracted interest due to its unusual physicochemical properties [18]. G–$C_3N_4$ is specifically divided into two cases of s–triazine–based $g-C_3N_4$ (SGCN) and tri–triazine–based $g-C_3N_4$ (TGCN). In 2014, a large crystalline thin films of SGCN had been fabricated by an ionothermal reaction [19]. The $g-C_3N_4$ exhibits a semiconductor characteristic with an approximately band gap of 2.70 eV. In 2015, nitrogenated holey graphene (NHG) with a stoichiometry of $C_2N$ in the plane was synthesized by a wet-chemical reaction [20]. The monolayer NHG consists of uniform periodic holes in a fused aromatic network structure, and exhibits a semiconductor behavior with an experimental band gap of 1.96 eV [21]. Thermal conductivity, mechanical properties, strain, atomic adsorption, and phononic characteristics of NHG have been investigated [21–24]. In 2017, single crystal $C_2N_3$ nanosheets were also synthesized by Miller [25]. It is observed that the emission wavelengths can be tuned by controlling the aggregation state of the nanosheets, which suggests that it has a potential application in the field of optoelectronic devices. Another form of graphitic carbon nitride with CN stoichiometry was also confirmed in experiment [26]. It is found that the monolayer CN is a semiconductor with the band gap value of 2.89 eV, and the band gap decreases to 2.75 eV as the number of layers increases [27].

In 2016, a new 2D polyaniline with a stoichiometry of $C_3N$ was successfully synthesized for the first time by carbonized organic single crystals. The experimental results show that $C_3N$ is a semiconductor with the band gap of 2.67 eV [28]. Mortazavi et al. investigated stiffness and thermal conductivity of $C_3N$ [13]. The result shows that $C_3N$ has remarkably high elastic modulus and thermal conductivity. Molecular dynamics simulations also show that it can withstand a high temperature of 4000 K. There exist disagreements between theoretical and experimental results for $C_3N$. For example, the experimental band gap of $C_3N$ is 2.67 eV, while the theoretical band gap is

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