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# Thermal properties of biased bilayer graphene and boron nitride nanoribbons

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ABSTRACT

The electronic structure, temperature-dependent thermal conductivity κ(T) and heat capacity $C_V$(T) of bilayer graphene nanoribbons (G/G), boron nitride nanoribbons (BN/BN) and graphene/boron nitride nanoribbons (G/BN) with AA and AB stacking are investigated using the tight binding model and Green's function method. The results show that the bilayer G/G with AA stacking is metallic independent of the bias while other structures with AA and AB stacking are semiconductor in absence of bias and their band gap reduce in the presence of bias. The κ(T) for all structures increases with temperature to its maximum value and then decreases by further temperature increasing. The κ(T) of bilayer BN/BN is smaller than that of bilayer G/G and G/BN. The $C_V$(T) of all structures increases up to a maximum value at $T = T_M$ (Schottky anomaly) and the corresponding $T_M$ value depends on the nanoribbons types and stacking as $T_M$(G/G) < $T_M$(G/BN) < $T_M$(BN/BN). The $C_v$(T) of bilayer G/G is larger than G/BN and BN/BN.

## 1. Introduction

During the past decade, two-dimensional (2D) materials have attracted great attention due to novel physical properties, such as mechanical, electronic and optical properties. In this context, graphene nanoribbons (GNRs) and boron nitride nanoribbons (BNNRs) exhibit the interesting properties due to their length width and edge structures. Nanoribbons are classified according to their edge structures into two groups, namely, armchair and zigzag nanoribbons. The nanoribbon width is defined by the number of dimer lines in the transverse direction [1].

In GNRs, their energy band gaps depend strongly on the ribbon edges and widths [2]. The zigzag GNRs (Z-GNRs) are always metallic with partial flat bands at Fermi level [3] whereas armchair GNRs (A-GNRs) are metallic ($N_a = 3m + 2$, where m is an integer) or semiconducting ($N_a = 3m$ and $N_a = 3m + 1$) depending on their width [4]. The boron nitride nanoribbons (BNNRs) are semiconductor with large band gap independent of their length and edges structure [5,6].

The application of the 2D based devices can be increased by controlling their electronic properties. The ability to control the electronic properties of 2D materials occurs by several methods such as strain, doping and electric fields and it makes these devices suitable candidates for electro optical applications. For the carbon nanotubes (CNTs) and boron nitride nanotubes (BNNRs) and nanoribbons, it has been shown that the electronic properties change by applying electric field [6–12]. For example, the band gap of BN nanotubes decreases linearly with transverse electric field until reaches zero [13]. Also, the modifications of electronic structure of GNRs and BNNRs occur with external electric field and the effects of electric field are more obvious in the BNNRs than that of GNRs [6]. These studies have been shown that in the strong enough field strength, the semiconductor metallic (and vice-versa) transition occurs [13–15].

In addition to applying the electric field, the bias also can change the electronic properties of these materials. Many studies on graphene like systems have been shown that the application of bias modifies the band gap of multilayers sheet and all changes in the band structure, directly reflect in their thermal and optical properties [16,17]. For example, the band gap of biased hexagonal BN graphene like multilayers decreases irrespective of the layer number and stacking manner [18]. Unlike to bilayer nanoribbons, many studies have been investigated the electronic properties of bilayer graphene and BN graphene like structures with density functional theory (DFT) and tight binding methods [19–21]. In this work, the electronic properties of GNRs and BNNRs has been investigated focusing attention on the effect stacking and bias. In addition to electronic properties, the study of thermal properties of low dimensional systems has attracted much interest due to the change the thermo-electronics properties of the devices with nano scale length.

Several studies have been investigated the thermal conductivity κ(T) of nanotubes and nanoribbons [22–26]. It has been shown that the CNTs have very high κ(T) comparable to in-plane graphite sheet [27]. For mono layer GNRs with various widths, it is found that the thermal

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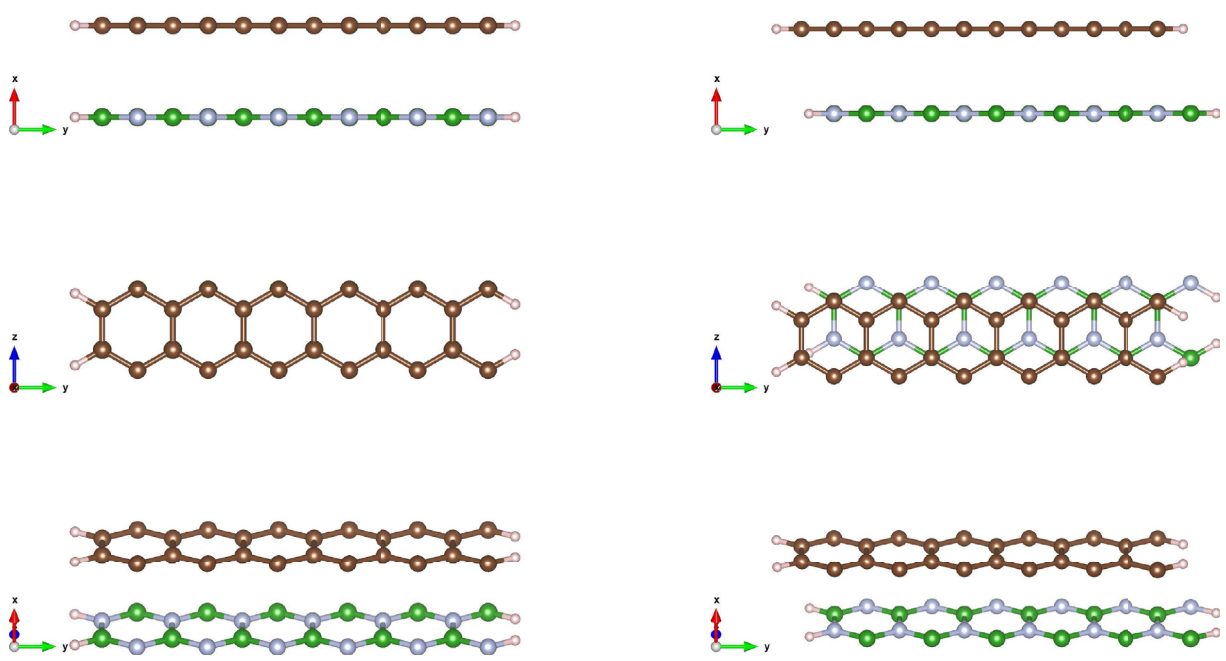

**Fig. 1.** Geometry structure of the bilayer GNR/BNNR with AA and AB stacking.

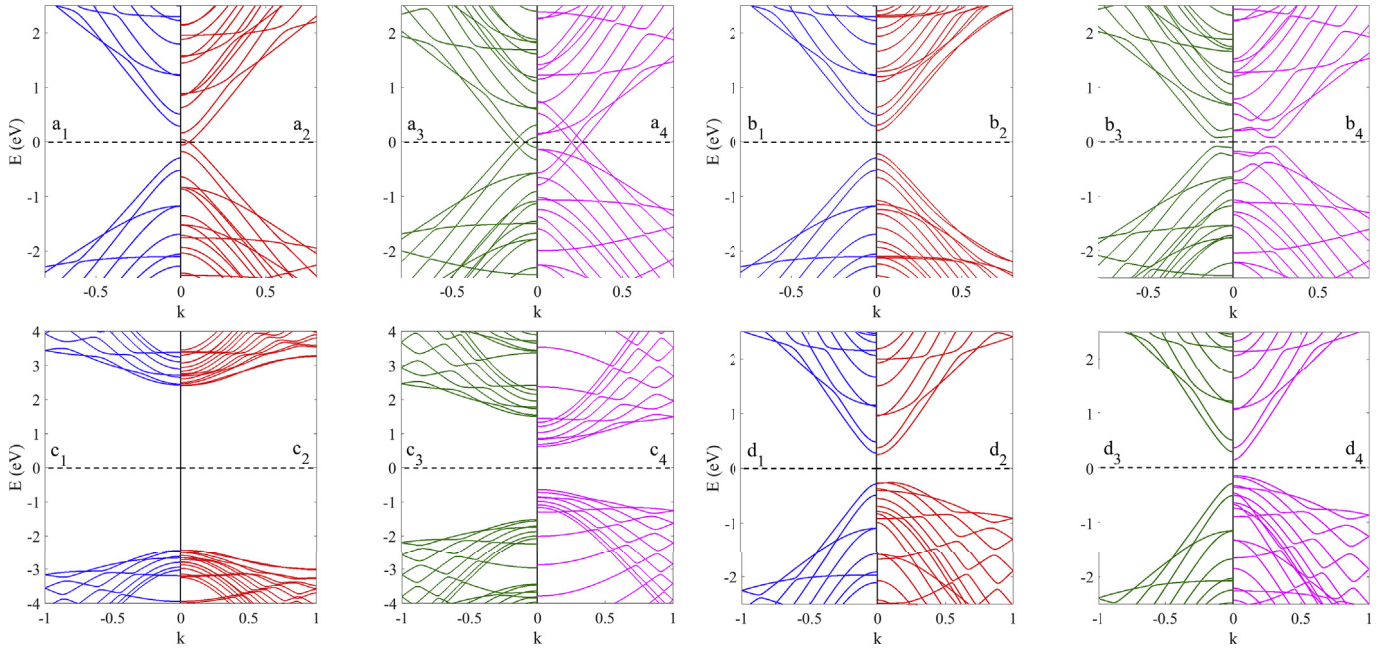


**Fig. 2.** Band structure of ($a_1$) and ($b_1$) monolayer GNR and bilayer AA stacking GNR/GNR in ($a_2$-$a_4$) U = 0, 1 and 2 eV and bilayer AB stacking GNR/GNR in ($b_2$-$b_4$) U = 0, 1 and 2 eV, respectively. Band structure of ($c_1$) monolayer BNNR and bilayer AA stacking BNNR/BNNR in ($c_2$-$c_4$) U = 0, 2 and 4 eV, respectively. Band structure of bilayer AA stacking GNR/BNNR ($d_1$.$d_2$) in U = 0 and 2.5 eV and bilayer AB stacking GNR/BNNR ($d_3$-$d_4$) in U = 0 and 2.5 eV, respectively.

conductivity decreases with width increasing due to the overlap between the non-hybridized pz orbitals [28]. The zigzag nanoribbons have appreciably larger thermal conductivity than the armchair nanoribbons due to the different phonon scattering rates at the armchair and zigzag edges [29]. By studying thermal transport of BNNRs with armchair and zigzag edge states, it has been shown that the κ(T) of zigzag-edged BNNRs is larger than that of armchair-edged nanoribbons at room temperature [30]. For symmetric GNRs, it is found that the calculated κ(T) is on the similar order of magnitude of the experimentally measured value for grapheme [29]. For GNRs, the thermal conductivity decreases by vacancies [29], tensile/compressive uniaxial strain [31] and the edge H-passivation [32]. Using nonequilibrium molecular dynamics method, it has been found that the κ(T) of multilayer GNRs monotonously decreases with the number of layers and the decreasing magnitude is proportional to the layer size, because the intensive phonon resonance increases by increasing the number of layers [33]. For the armchair GNRs it has been found that the third-order conductance exhibits a strong Fermi level dependence at low temperatures [34]. The phonon frequency dependence of thermal conductivity is investigated for GNRs and the results showed that they could have great potentials for thermoelectric applications [35]. The κ(T) of BNNRs is respectively predicted to be one order of magnitude less than those of graphene and zigzag BNNRs have a higher thermal conductivity than armchair BNNRs [36]. Beyond armchair and zigzag