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Bor arsenit bazlı nano-transistörlerde elektrot genişliğinin enerji aralığı üzerindeki etkisinin incelenmesi, bir DFT çalışması

Investigating the width effect on energy gaps of electrodes in boron arsenide based nano-transistors, a DFT study

Nilüfer Ertekin[1,*]

[1] *Yalova Üniversitesi, Elektrik elektronik Mühendisliği Bölümü, Yalova, Türkiye*

Abstract

This study deals with electronic properties of Boron Arsenide nanoribbons using Density function theory (DFT) calculations. Under specific conditions, nanoribbons can be used as Nano-transistors. It is feasible to modify nanoribbons' electronic properties, such as bandgap and conductivity, by varying their width and edge shape. Source, drain, and gate are basic parts of a conventional field-effect transistor (FET). The channel's conductivity can be changed by applying a voltage to the gate electrode. In current research, Boron Arsenide nanoribbons has been investigated as lead electrode of a transistor and stability of the sheet has been confirmed by positive phonon vibrational modes. Utilizing the band structure spectrum, band gap as an electronic property is measured and reported. Different width values for electrodes have been considered and it has represented that the band gap is size dependent and increasing in ribbon's size to bulk structure, results in decrements in band gap energy value

Keywords: Nano-transistor, BAs Nanoribbon, Band gap, Armchair edge, Density function theory (DFT)

Öz

Bu çalışma, Yoğunluk Fonksiyon Teorisi (DFT) hesaplamalarını kullanarak Boron Arsenit nanoşeritlerin elektronik özellikleri araştırılmıştır. Belirli koşullar altında, nanoşeritler Nano-transistör olarak kullanılmaktadır. Şeritlerin genişliği ve kenar şeklini değiştirerek, nanoşeritlerin bant aralığı ve iletkenliği gibi elektronik özellikleri değiştirilebilir. Source, drain, ve gate, geleneksel bir alan etkili transistörün (FET) temel parçaları olarak tanımlanır. Kanalın iletkenliği, kapı elektroduna bir gerilim uygulayarak değişmektedir. Bu araştırmada Boron Arsenide nanoşeritleri bir transistörün lead elektrotu olarak kullanımı incelenmiştir ve tabakaların kararlılıkları pozitif fonon titreşim modları ile doğrulanmıştır. Band yapısı spektrumu kullanılarak, elektronik özelliği olarak bant aralığı ölçülüp, rapor edilmiştir. Elektrotlar için farklı genişlik değerleri kullanarak bant aralığının boyuta bağlı olduğu ve şeridin boyutunun artmasıyla bant aralığı enerji değerinde azalmaya yol açtığı gösterilmiştir.

Anahtar kelimeler: Nano-transistör, BAs Nanoribon, Bant aralığı, Armchair kenar, Yoğunluk fonksiyonu teorisi (YFT)

1 Introduction

A nano-transistor is a transistor made from extremely small materials. These fundamental elements of modern electronic technology are studied and developed with the goal of controlling the flow of electrical current. To enhance performance and increase the number of transistors that can be packed onto a chip, traditional transistors, also known as metal-oxide-semiconductor field-effect transistors (MOSFETs), have had their size decreased during a period of several decades. This miniaturization is carried to the nanoscale by nano-transistors, which have dimensions on the order of nanometres. The development of two-dimensional (2D) materials including graphene [1], h-BN [2], transition-metal dichalcogenides (TMDC) [3-4], and more [5-11] has brought about a great deal of interest in the field of nanoscience and technology. They can be utilized to create smaller and faster field-effect transistors. The lower carrier mobility and lack or large band gap of these materials [12-13], however, restrict their field of application, necessitating more research into alternate materials with a wider range of applications [14].

Boron arsenide (BAs) is a compound made up of boron (B) and arsenic (As) atoms. It is a semiconductor element with special qualities that make it appealing for a variety of applications. In addition, Boron arsenide (BAs) nanoribbons are thin ribbons or strips with a width measured in nanometers. They are one-dimensional nanostructures that have received interest owing to their distinctive electronic and thermal characteristics [15-18].

BAs nanoribbons may have metallic behavior or be semiconducting with a bandgap, depending on the width and type of edge and this property make them potential candidates for nano-electronic devices, including field-effect transistors (FETs), sensors, and nanoscale logic circuits. Armchair nanoribbons contain edges that, by being parallel to the crystal's lattice vectors, present a zigzag pattern. The name "armchair" comes from the zigzag pattern's resemblance to an armchair's arms.

The electronic characteristics of armchair nanoribbons depend on their width and the characteristics of the material they are formed of [18-19]. It is important to note that BAs nanoribbons are still in their early years, and additional study

* Sorumlu yazar / Corresponding author, e-posta / e-mail: nilüfer.ertekin@yalova.edu.tr (N. Ertekin)
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is required to completely comprehend their properties, production processes, and prospective applications.

Based on the above-mentioned details, in the current study, we investigated the effect of BAs nanoribbons as the lead electrodes in nano-transistors by employing first-principles density functional theory (DFT)- based periodic calculations. A pure BAs sheet was made and the system relaxed and reached its minimum energy.

In the following structure, stability is checked by phonon distribution, and Band structure is calculated for optimized structure specifically. After developing the lead electrode from the structure, the effect of different values of width in the bandgap of the electrode has been investigated using band structure and density of function dispersions. Understanding the electronic properties of materials requires an understanding of the band structure and density of states (DOS), two fundamental concepts in DFT.

One of the most fundamental and important properties of a crystalline solid is its electronic band structure. The exact estimation of electronic band structures is an essential problem of computational condensed matter physics [20].

DOS diagrams present an easy way to characterize advanced electronic structures. It is a simple and useful way to determine the electronic structure of a material. Section 2 describes computational details and the result of our approach is described in Section 3.

2 Computational details

In this study the analysis has been performed by DFT-based periodic calculations, using the Quantum Espresso Package. A BAs sheet with a hexagonal structure was considered. Electronic structure calculations and geometry optimizations including lattice constant and atomic positions are done based on an iterative solution of the Kohn-Sham equation [21] and ultra-soft Pseudopotentials by minimizing the total energy.

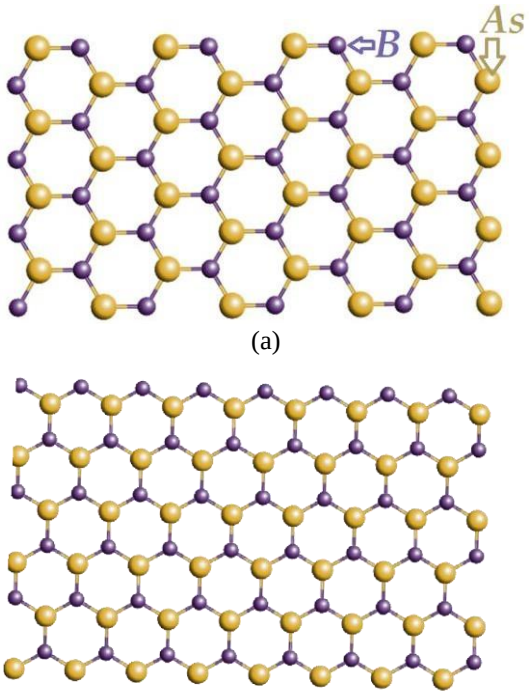
There are two fundamental types of nanoribbons: those with armchair-style edges and those with zigzag edges. Both structures are depicted schematically for BAs in Figure 1. The direction of these edges within the sheet varies by 30°. In this study, the armchair edge was modeled and all dangling bonds were terminated by hydrogen atoms Following, nanoribbons of various widths were created, their electronic properties were obtained, and they were compared to one another based on their gap energies.

Both valence band maximum (VBM) and conduction band minimum (CBM) details are extracted and reported

3 Results and discussions

Pristine Boron Arsenide structure was created and has been exposed in Figure 2a and optimized and the convergence limits for energy, forces, and stress were reached -26.7 Ry, 0 Ry/Bohr, and 0.21 kBar respectively.

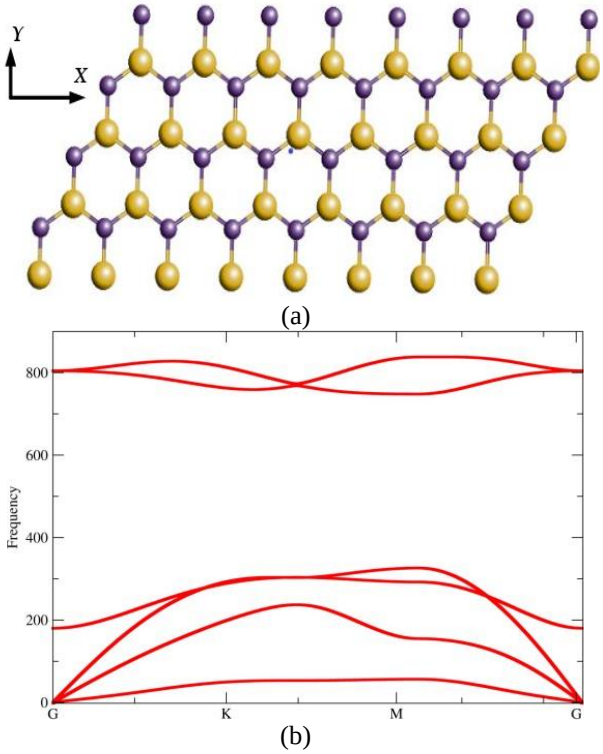
For investigating the dynamical stability of materials, phonon calculations are an appropriate technique in general. The phonon spectrum provides information about the frequencies and wave vectors associated with quantized lattice vibrations. The phonon spectrum of the modeled structure has been shown in Figure 2b. The phonon dispersion is along Γ-M -K -Γ within the Brillouin zone and there were no imaginary frequencies in phonon dispersion, this means the structure's dynamic stability and the system is in local minimum energy.



(a)

(b)

Figure 1. a- Armchair-style edge b- Zigzag-style edge of BAs sheet



(a)

(b)

Figure 2. (a)- structure (b)- phonon spectrum of BAs sheet

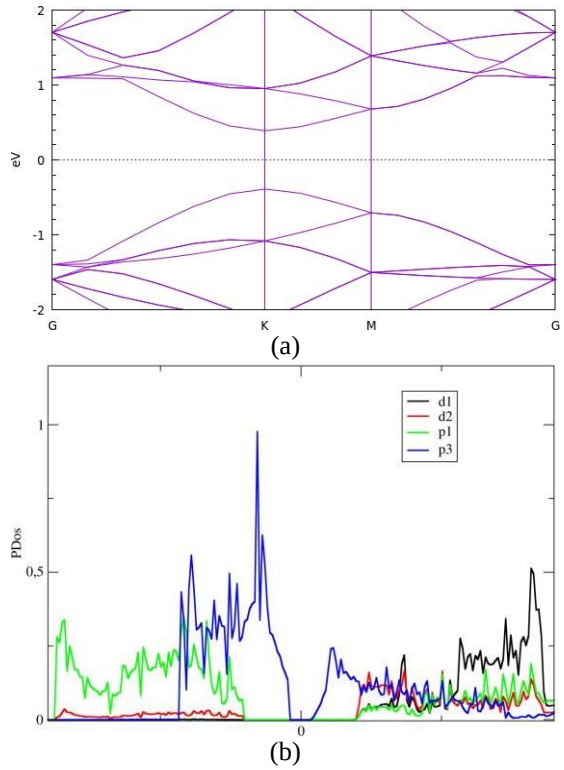


Figure 3. (a)- The energy band structure diagram (b)- DOS of pristine BAs sheet

The energy band structure and density of states diagrams of pristine BAs sheet have been shown in Figures 3a, and 3b. The band gap is 0.76, as can be seen in Figure 3a,which is consistent with earlier studies [14]. The conduction band minimum value of the structure also corresponds with the valence band maximum value at the K point of the Brillouin zone. it is a direct band gap and VBM and CBM energies are 0.38 and -0.38 respectively. The density of state dispersion of the system was exposed in Figure 3b. It represents the distribution of available electronic states as a function of energy. The width of an armchair nanoribbon, which defines the number of atomic rows in the ribbon, affects the specific form and properties of the band structure.

In the current research, we investigated the effect of width on nanoribbons with 13Å, 17Å, 23Å, and 47Å widths respectively. Figure 4 represented the structure of nanoribbons and their band structures with different widths. The electrodes with 13Å, 17Å, 23Å, and 47Å width represented 0.96, 0.88, 0.86, and 0.78 gap energies respectively. Figure 5 depicts the band gaps produced for the various width ABsNRs and GNR. Table 1 summarizes the energy of the band gap, valence, and conduction bands for an accurate representation of the total data.

It was understood from the table and figures that, as the width of the nanoribbon gets larger the band gap of the electrode slowly narrows related to the quantum confinement effect. As the ribbon width decreases, quantum confinement becomes more significant, and the electronic states become more localized. This confinement can lead to an increase in the band gap, making narrower nanoribbons more likely to exhibit semiconducting behavior [23, 24]

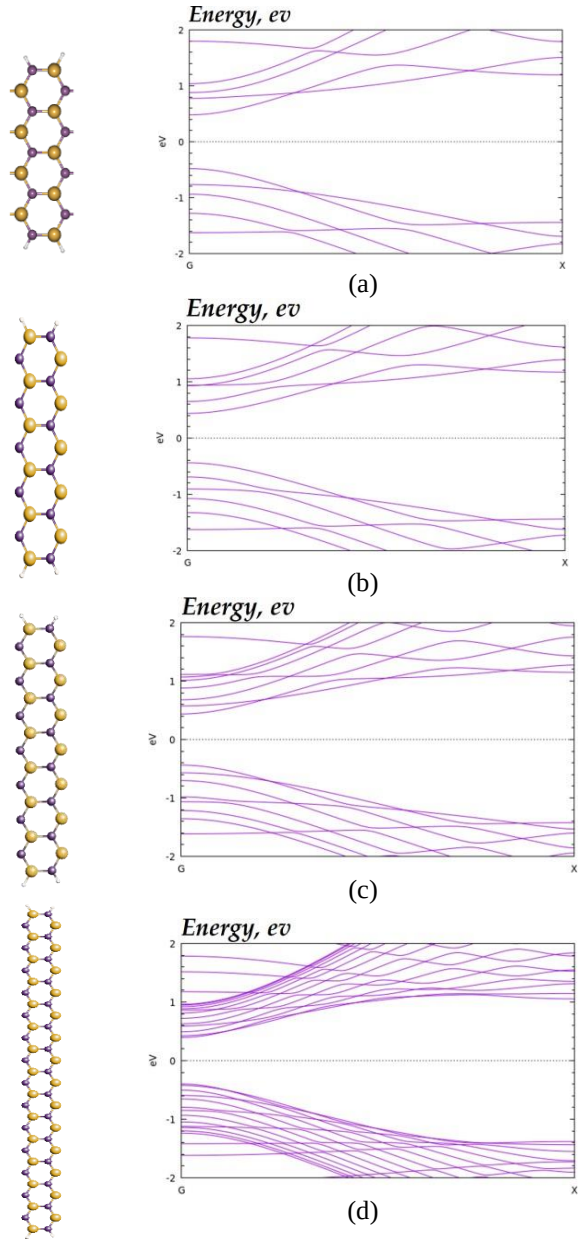


Figure 4. BAs nanoribbons with different width andtheir band structure spectrums

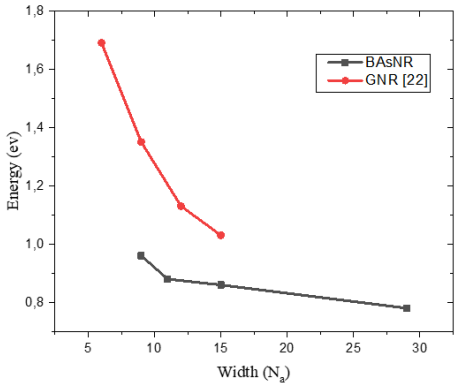


Figure 5. Band gaps according to the varying width for BAsNR and GNR.

Table 1. The band gap, valence, and conduction bands ofdifferent widths of the nanoribbons

	This work				Other works (Armchair graphene nanoribbon)		
Structure	Width (Å)	VB (eV)	CB (eV)	Band gap (eV)	Structure	Band gap (eV)	Ref.
9-aBAsNR	13	-0.48	0.48	0.96	6-aGNR	1.69	[22]
11-aBAsNR	17.5	-0.44	0.44	0.88	9-aGNR	1.35	[22]
15-aBAsNR	23	-0.43	0.43	0.86	12-aGNR	1.13	[22]
29-aBAsNR	47	-0.39	0.39	0.78	15-aGNR	1.03	[22]

The source and drain electrodes in a nano-transistor, commonly referred to as the leads, have a significant impact on how the transistor operates and its performance. The characteristics and arrangement of these leads can shape the transistor's behavior. The width of these leads is particularly important because it determines how much current the transistor can handle and how efficiently it conducts electricity. Increasing the width of nanoribbons can increase the mobility of electrons [18, 25], and this can influence the performance of the leads and the transistor. While wider leads can facilitate larger currents, they can also introduce unwanted side effects, such as increased capacitance and resistance, which might influence the speed of switching and the power usage of the transistor.

4 Conclusions

Using DFT and Quantum ESPRESSO package [15], the geometrical, electronic, and phonon calculation of BAs sheets were performed, and as nano-transistor electrodes, nanoribbon structures with different widths were extracted from the sheet. The electronic calculations represented that the proposed BAs material is a semiconductor with a direct band gap which has below 1ev gap energy, making it an appropriate choice for nano-transistor applications. The result showed that by decreasing in width, the band gap increased and the band gap is a size-dependent subject. This is due to quantum confinement and the electronic states become more concentrated as the ribbon width gets smaller. The band gap could expand because of this limitation. The width of source and drain electrodes in a nano-transistor, often called leads, is a critical factor in determining the transistor's current-carrying capacity and efficiency. Widening nanoribbons can improve electron mobility, which affects both lead and transistor performance, but wider leads can introduce unwanted effects like increased capacitance and resistance, potentially influencing switching speed and power usage.

Conflict of interest:

The author declares that there is no conflict of interest.

Similarity rate (iThenticate): %4

References

[1] A. K. Geim, and K. S. Novoselov, The Rise of Graphene. Nature Materials, 6, 183- 191, 2007. https://doi.org/10.1038/nmat1849.

[2] L. Song *et al*., Large Scale Growth and Characterization of Atomic Hexagonal Boron Nitride Layers. Nano Lett. 10, 3209- 3215, 2010. https://doi.org/ 10.1021/nl1022139.

[3] J.A Wilson and A.D. Yoffe, The transition metal dichalcogenides discussion and interpretation of the observed optical, electrical, and structural properties, Advances in Physics, 18:73, 193335, 1969. https://doi.org/ 10.1080/00018736900101307.

[4] S. Manzeli, D. Ovchinnikov and D. Pasquier, 2D transition metal dichalcogenides. Nat Rev Mater, 2, 17033, 2017. https://doi.org/10.1038/natrevmats.2017.33.

[5] A. Zhou *et al*., From structural ceramics to 2D materials with multi-applications: A review on the development from MAX phases to MXenes. J Adv Ceram 10, 1194–1242, 2021. https://doi.org/10.1007/s40145-021 0535-5.

[6] M. Xu, T. Liang, M. Shi, and H. Chen, Chemical Reviews, 113 (5), 3766-3798, 2013. https://doi.org/10.1021/cr300263a.

[7] M. Mathew *et al*., A review on mechanisms and recent developments in p-n heterojunctions of 2D materials for applications. J Mater Sci 56, 9575–9604, 2021. https://doi.org/10.1007/s10853-021-05884-4

[8] P. Miro, M. Audiffred, and T. Heine, An Atlas of Two-Dimensional´ Materials. Chem. Soc. Rev. 43, 6537−6554, 2014. https://doi.org/10.1039/C4CS00102H

[9] V.S. Pratik, T. Anjana, T. Ranjit and S.R. Chandra, Nanoribbons of 2D materials: A review on emerging trends, recent developments and future perspectives, Coordination Chemistry Reviews, 453, 214335,2022. https://doi.org/10.1016/j.ccr.2021.214335.

[10] S. Zhang *et al.*, Atomically Thin Arsenene and Antimonene: Semimetal- Semiconductor and IndirectDirect Band-Gap Transitions. Angewandte.

Chemie, Int. Ed. 54, 3112− 3115, 2015. https://doi.org/10.1002/anie.201411246

[11] S. Zhang *et al*., Antimonene Oxides: Emerging Tunable Direct Bandgap Semiconductor and Novel Topological Insulator. Nano Lett. 17, 3434−3440 2017. https://doi.org/10.1021/acs.nanolett.7b00297

[12] F. Xia, D. B. Farmer, Y. M. Lin and P. Avouris, Graphene Field Effect Transistors with High on/off Current Ratio and Large Transport Band Gap at Room Temperature. Nano Lett. 10, 715718, 2010. https://doi.org/10.1021/nl9039636

[13] G. He, *et al.* Conduction Mechanisms in CVD-Grown Monolayer MoS2 Transistors: From Variable-Range Hopping to Velocity Saturation. Nano Lett. 15, 5052−5058, 2015. https://doi.org/10.1021/acs.nanolett.5b01159

[14] M. Kamaraj and V. Subramanian, Exploring Multifunctional Applications of Hexagonal Boron Arsenide Sheet: A DFT Study ACS Omega, 3, 9533-9543, 2018. https://doi.org/10.1021/acsomega.8b00946.

[15] H. Shan., Q. He, X. Luo and Y. Zheng, First-Principles Calculations of Monolayer h-BN Nanosheets and Nanoribbons with Ultrahigh Phonon-Limited Hole Mobility for Wide Band Gap P-Channel Transistors. The Journal of Physical Chemistry C, 127, 9278-9286, 2023. https://doi.org/10.1021/acs.jpcc.3c00349

[16] J. Cao, et al., On functional boron nitride: Electronic structures and thermal properties, Materials Today Electronics, 2, 100005, 2022. https://doi.org/10.1016/j.mtelec.2022.100005.

[17] T. Miao., M. Xiang, D. Li, X. Wang, Electrical and thermal transport properties of high crystalline PdTe2 nanoribbons under a strong magnetic field – Nanoscale, 14, 10101-10107, 2022. https://doi.org/10.1039/D2NR02049A

[18] D. Yulan *et al*., First-principal prediction of the electronic property and carrier mobility in boron arsenide nanotubes and nanoribbons. Journal of Applied Physics 28, 124303, 2019. https://doi.org/10.1063/1.5110868

[19] N.M. Díez *et al.,* Width-Dependent Band Gap in Armchair Graphene Nanoribbons Reveals Fermi Level Pinning on Au (111) ACS Nano, 11, 11661-11668, 2017. https://doi.org/10.1021/acsnano.7b06765.

[20] N.R. Knøsgaard, and K.S. Thygesen, Representing individual electronic states for machine learning GW band structures of 2D materials. Nat Commun 13, 468, 2022. https://doi.org/10.1038/s41467-022-28122-0.

[21] W. Kohn and L. J. Sham, Self-Consistent Equations Including Exchange and Correlation Effects, Phys. Rev., 140.A1133, 1965. https://doi.org/10.1103/PhysRev.140.A1133

[22] N. Merino-Díez, *et al.*, Width-dependent band gap in armchair graphene nanoribbons reveals Fermi level pinning on Au (111). ACS nano, 11, 11661-11668. https://doi.org/10.1021/acsnano.7b06765

[23] G. Kalosakas, N.N. Lathiotakis, and K. Papagelis, Width dependent elastic properties of graphene nanoribbons. Materials, 14, 5042, 2021. https://doi.org/10.3390/ma14175042

[24] S. Dutta, and S. K. Pati, Novel properties of graphene nanoribbons: a review. Journal of Materials Chemistry, 20, 8207-8223, 2010. https://doi.org/10.1039/C0JM00261E

[25] B. Zeng *et al.*, First-principles prediction of the electronic structure and carrier mobility in hexagonal boron phosphide sheet and nanoribbons. The Journal of Physical Chemistry C, 120(43), 25037-25042, 2016. https://doi.org/10.1021/acs.jpcc.6b07048