

Research Article

Geometry, Energy, and Some Electronic Properties of Carbon Polyprismanes: *Ab Initio* and Tight-Binding Study

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We report geometry, energy, and some electronic properties of $[n,4]$ - and $[n,5]$ prismanes (polyprismanes): a special type of carbon nanotubes constructed from dehydrogenated cycloalkane C_4 - and C_5 -rings, respectively. Binding energies, interatomic bonds, and the energy gaps between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) have been calculated using density functional approach and nonorthogonal tight-binding model for the systems up to thirty layers. It is found that polyprismanes become more thermodynamically stable as their effective length increases. Moreover, they may possess semiconducting properties in the bulk limit.

1. Introduction

Carbon $[n,m]$ prismanes (polyprismanes) can be regarded as stacked layers of dehydrogenated cycloalkane molecules, where m is the number of vertices of the closed carbon ring and n is the number of layers [1]. However, the polyprismanes' ends are passivated by hydrogen atoms to avoid the dangling bonds. For large n , polyprismanes (PP) represent single-walled carbon nanotube analogs with an extremely small cross-section as a regular polygon. Despite the fact that PP are of considerable fundamental and practical interest, their synthesis is very difficult task due to their high-strained carbon frame. Unlike carbon nanotubes, polyprismanes have rectangles on their surfaces instead of hexagons. So the angles between covalent C–C bonds are different from the value 109.5° usual for the sp^3 -hybridized carbon orbitals. Only "simplest" PP representatives are obtained: $[2,3]$ prismane C_6H_6 (Ladenburg's prismane) [2], $[2,4]$ prismane C_8H_8 (hydrocarbon cubane) [3], and $[2,5]$ prismane $C_{10}H_{10}$ [4]. Attempts to synthesize $[2,m]$ prismanes starting from $[2,6]$ prismane $C_{12}H_{12}$ failed. Nevertheless, hypothetical

ways of synthesis based on high-level density functional calculations are predicted for $[3,4]$ prismanes and $[4,4]$ prismanes [1]. Moreover, structural characteristics and electronic properties of $[n,m]$ prismanes with $n = 2$, $m = 6 \div 18$ [5]; $n = 4$, $m = 3 \div 6$ [6]; $n = 2 \div 16$, $m = 6$ [7, 8] are actively studied in terms of the density functional theory. The evolution of aromaticity along the thermally forbidden $[4 + 4]$ and $[6 + 6]$ dimerizations of cyclobutadiene and benzene to give $[2,4]$ prismane and $[2,6]$ prismane, respectively, is also discussed in the literature [9]. The special place is occupied by investigations of mechanical properties of polyprismanes, including the analysis of the edge doping (by replacing hydrogen atoms with chemical functional groups or radicals) influence on the PP mechanical characteristics [10, 11]. It is established that polyprismanes are molecular auxetics, that is, compounds having negative Poisson's ratio [12]. In addition, high kinetic stability of small prismanes (namely, $[2,6]$ prismanes and $[2,8]$ prismanes) is also confirmed via direct molecular dynamics simulations [13]. Long $[n,m]$ prismanes with the large values of n are of special interest. They are considered as molecular wires for nanoelectronic applications

[14]. In addition, recent *ab initio* calculations predicted that “long” (up to $n = 10$) and even infinite ($n \rightarrow \infty$) $[n,4]$ prismanes were stable and could exhibit the metallic behavior [15]. Moreover, the particular electronic properties of long PP make them potentially suitable in the biomedical sector as biological ion carriers [16–18]. So they can be used as drug delivery systems in the field of nanomedicine. But despite series of evident achievements in physical chemistry of long PP, their geometry, energy, and electronic properties are not well studied.

Nevertheless, PP are quite promising compounds. For example, polyprismanes can be functional nanowires with controlled electronic characteristics and can be used in computational logic elements. The incorporation of metastable carbon-nitrogen structures (nitrogen chains) inside the higher PP can stabilize the latter, which will make it possible to obtain an efficient high-energy material. The same principle of the formation of endohedral complexes (the encapsulation of therapeutic preparations inside polyprismanes) can be used for developing drug delivery systems. The use of PP as elements of measuring equipment, such as probes (tips) of the atomic-force microscopes, is also urgent. The absence of free covalent bonds makes polyprismanes insensitive to contaminants of the external medium (free radicals), which lowers the reaction ability of the tip making it possible to attain atomic resolutions in a microscope. All these possible applications pose quite concrete questions for the researchers: what are the limiting operating temperature modes of materials based on PP; how can we estimate lifetimes of the samples in extreme conditions (e.g., at cryogenic temperatures); how will electronic characteristics vary (e.g., conductivity) with an increase in the efficient sample length; how will edge doping affect their mechanical properties; and finally what compounds from the PP family are most thermodynamically and kinetically stable and the most probable candidates for the practical use?

In this paper, we present density functional theory and tight-binding calculations for the $[n,4]$ - and $[n,5]$ prismanes’ family with $n = 2 \div 30$. The main purpose of this work is to obtain their binding energies, interatomic bonds, and HOMO-LUMO gaps and to analyze the behavior of these values in the bulk limit ($n \rightarrow \infty$). We hope that our study will stimulate the subsequent theoretical and experimental research of PP.

2. Materials and Methods

In our study we use density functional theory as well as the nonorthogonal tight-binding model (NTBM) [20]. Density functional theory (DFT) with Becke’s three-parameter hybrid method and the Lee-Yang-Parr exchange-correlation energy functional (B3LYP) [21, 22] with the electron basis set of 6-311G(d) [23] were used to optimize the geometries and obtain the structural, energy, and electronic (namely, HOMO-LUMO gaps) characteristics of the polyprismanes. The geometries of all polyprismanes were optimized using the GAMESS program package [24]. In the tight-binding model, the total potential energy of the system is the sum of

the quantum-mechanical electronic energy and the “classical” ionic repulsive energy. The former is defined as the sum of one-electron energies over the occupied states, the energy spectrum being determined from the stationary Schrödinger equation ($2S$, $2P_x$, $2P_y$, and $2P_z$ orbitals of carbon atoms and $1S$ orbitals of hydrogen atoms are considered). The electronic Hamiltonian is calculated from overlap matrix elements using extended Hückel approximation [25] with Anderson distant dependence for Wolfsberg-Helmholtz parameter [26]. The overlap integrals are calculated using standard Slater-Koster-Roothaan procedure [27, 28]. Therefore, the analytical expressions for the overlap integrals greatly simplify the calculation of Hamiltonian. The parameters’ fitting of tight-binding model is based on the criterion of the best correspondence between the computed and experimental (not derived from *ab initio* calculations) values of binding energies, bond lengths, and valence angles of several selected small hydrocarbon molecules (for parameterisation details, see [20, 29]). To validate the model developed, we computed the binding energies, bond lengths, and valence angles for various H–C–N–O compounds not used in the fitting procedure and compared them with the experimental data from NIST database [19]. The resulting tight-binding potential is well suited to modeling various $H_k C_l N_m O_n$ molecules from small clusters to large systems as graphene, diamond, peptides, polyprismanes, and so forth [20]. For example, NTBM binding energies and structural properties for peptides such as bradykinin and colistin are in good agreement with the corresponding DFT calculations [20]. Unfortunately, we are not aware of experimental data derived for any polyprismane, except for cubane C_8H_8 . For cubane, NTBM model is in excellent agreement with the existent experimental data. For example, experimental C–C and C–H bond lengths are 1.570 and 1.082 Å, respectively, and NTBM model gives 1.571 and 1.097 Å, respectively [30]. Binding energy obtained within the NTBM model (4.42 eV/atom) is also in good agreement with the experimental value (4.47 eV/atom) [30]. In addition, earlier we calculated the binding energies for hexa- and octaprismanes using NTBM and DFT/B3LYP/6-311G levels of theory. The binding energies of hexaprismane and octaprismane in terms of NTBM model were 4.56 and 4.47 eV/atom, respectively. These results agree well with our data found using the DFT/B3LYP/6-311G: 4.50 and 4.40 eV/atom for hexaprismane and octaprismane, respectively [13]. It should be noted that *ab initio* methods (say density functional theory) are very accurate but computer-resources demanding and hence applicable to small systems only. Calculation time within the DFT approach is estimated as $\sim N^4 \div N^5$, where N is the number of atoms in molecular system. To check the convergence of the binding energies and the HOMO-LUMO gaps of “long” polyprismanes, we considered the molecular systems up to 500 carbon atoms. So the geometry and energy optimization of such systems in the frame of DFT is very computer resource-intensive or impossible. Therefore, the tight-binding approach is rather good compromise between the accuracy and computational costs and is commonly used for quantum chemistry modeling, including the calculation of binding energies, bond lengths, valence angles, and HOMO-LUMO gaps [31–33].

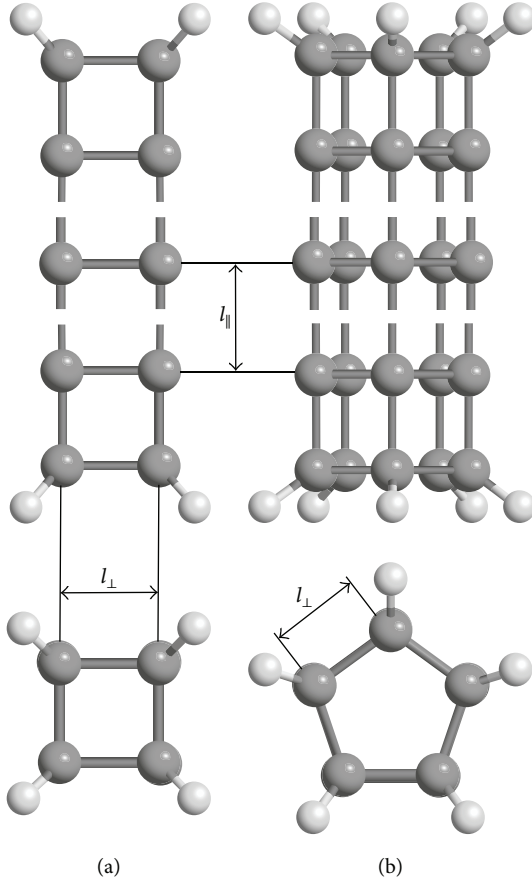


FIGURE 1: Structures of the (a) $[n,4]$ - and (b) $[n,5]$ prismanes. Top-side view, bottom-top view. Symbols l_{\parallel} and l_{\perp} correspond to interlayer and intralayer C–C bonds, respectively.

The samples studied are $[n,m]$ prismanes with $m = 4$ and 5 (tetra- and pentaprismanes, resp.) and $n = 2 \div 30$ (see Figure 1). To obtain the equilibrium structures of polyprismanes, we used the method of structural relaxation so that the corresponding initial configuration relaxed to a state with the local or global energy minimum under the influence of intramolecular forces only. First of all, the forces acting on the all atoms were calculated using the Hellmann-Feynman theorem [34]. Next, atoms were shifted in the direction of the forces obtained proportional to the corresponding forces. Then, the relaxation step was repeated. The whole structure is relaxed up to residual atomic forces smaller than 10^{-4} eV/Å.

Note that for all polyprismanes studied we also calculated the frequency spectra in the framework of the same level of theory after the geometry optimization. All frequencies were positive for each metastable configuration.

3. Results and Discussion

3.1. Geometrical Parameters. For the all PP we studied it is possible to distinguish two different types of carbon–carbon covalent bonds (see Figure 1): parallel to polyprismane main axis interlayer C–C bonds (l_{\parallel}) and perpendicular to main

TABLE 1: Bond lengths of various $[n,4]$ prismanes obtained within the NTBM model. Experimental values for $[2,4]$ prismane (cubane) are given in parentheses [19]. All bond lengths are quoted in angstroms.

Bond	n		
	2	30	∞
l_{\parallel}	1.570 (1.571)	1.541 \div 1.561	1.541
l_{\perp}	1.570 (1.571)	1.593 \div 1.642	1.641
l_{CH}	1.082 (1.097)	1.084	—

TABLE 2: Bond lengths of various $[n,5]$ prismanes calculated within the NTBM model. Results obtained for $[2,5]$ prismane (pentaprismane) within DFT/B3LYP/6-311G(d) are given in parentheses. All bond lengths are quoted in angstroms.

Bond	n		
	2	30	∞
l_{\parallel}	1.601 (1.571)	1.560 \div 1.592	1.561
l_{\perp}	1.538 (1.560)	1.563 \div 1.611	1.610
l_{CH}	1.086 (1.091)	1.087	—

axis intralayer C–C bonds (l_{\perp}). Their characteristic values for $[n,4]$ - and $[n,5]$ prismanes with $n = 2, 30$ and in the bulk limit are presented in Tables 1 and 2 for $[n,4]$ - and $[n,5]$ prismanes, respectively.

The ranges of bond lengths for $[30,4]$ - and $[30,5]$ prismanes are caused by the edge effects including C–H interactions. That is why the C–C bonds near the polyprismanes edge are longer than in the center. Optimized bond distances indicate that the interlayer C–C bonds in the “long” PP are shorter than the intralayer ones. This may be caused by the nonequivalence of p -orbitals spatial distribution of neighboring carbon atoms along and across the main axis of polyprismane. Thus, it leads to redistribution of electronic density, which defines the formation of two types of covalent bonds in polyprismane. It is interesting to notice that l_{\parallel} bond lengths in “simple” prismanes are quite longer than corresponding lengths in the bulk limit. As for l_{\perp} bond lengths, the reverse trend is observed: C–C bonds in “simple” prismanes are shorter than corresponding ones in the bulk limit. Note that C–H bond lengths depend slightly on the effective length of PP.

3.2. Size Dependence of the Binding Energies and the HOMO-LUMO Gaps. The binding energies of $[n,4]$ - and $[n,5]$ prismanes C_lH_k are calculated by the equation

$$E_b [\text{eV/atom}] = \frac{1}{N_{\text{at}}} \{kE(\text{H}) + lE(\text{C}) - E_{\text{tot}}(\text{PP})\}, \quad (1)$$

where $N_{\text{at}} = k + l$ is the total number of atoms in the polyprismane, $E(\text{C})$ and $E(\text{H})$ are the energies of isolated carbon and hydrogen atoms, respectively, and $E_{\text{tot}}(\text{PP})$ is the total energy of the corresponding polyprismane. The polyprismane with higher binding energy E_b (lower potential

TABLE 3: Binding energies E_b and HOMO-LUMO gaps Δ_{HL} for various $[n, 4]$ prismanes calculated within the NTBM model and at DFT/B3LYP/6-311G(d) level of theory.

n	E_b , eV/atom		Δ_{HL} , eV	
	NTBM	DFT/B3LYP/6-311G(d)	NTBM	DFT/B3LYP/6-311G(d)
2	4.42	4.52	5.92	8.35
3	4.51	4.56	3.55	4.59
4	4.59	4.62	3.19	3.48
5	4.65	4.68	2.87	3.37
6	4.69	4.71	2.70	3.23
7	4.73	4.73	2.61	2.91
8	4.75	4.76	2.51	2.78
9	4.78	4.77	2.44	2.71
10	4.79	4.79	2.40	2.69

energy) is more thermodynamically stable and vice versa. HOMO-LUMO gap is defined as energy gap between the highest occupied molecular orbital and the lowest unoccupied molecular orbital. The binding energies E_b and the HOMO-LUMO gaps Δ_{HL} obtained for small $[n, 4]$ prismanes ($n = 2 \div 10$) are summarized in Table 3.

Figure 2 displays the binding energies E_b and the HOMO-LUMO gaps Δ_{HL} of the $[n, 4]$ prismanes, for the larger n .

Thus, we calculated E_b and Δ_{HL} within the DFT approach for shorter PP ($n = 2 \div 10$) and using NTBM method for longer ones ($n = 7 \div 30$). According to our calculations, NTBM model systematically underestimates the value of Δ_{HL} compared with DFT (see Table 3). It should be noted that tight-binding methods usually underestimate the value of the HOMO-LUMO gap of a few tenths of eV compared to DFT [35, 36]. Therefore, we shifted all HOMO-LUMO gaps obtained via the NTBM by 0.35 eV. From the overlapping area on Figure 2, one can see that the accuracy of the resulting NTBM is in good agreement with the DFT. Thus, the NTBM model is suitable to the calculation of the energy and electronic characteristics of PP.

For $[n, 4]$ prismanes, we found that E_b and Δ_{HL} depend linearly on n^{-1} (here we do not take into consideration point with $n = 2$, which corresponds to the cubane C_8H_8 molecule due to its abnormal behavior; e.g., HOMO-LUMO gaps obtained within NTBM and DFT vary greatly). The corresponding analytical forms are

$$\begin{aligned} E_b(n) &= 4.9 - 1.2n^{-1}, \\ \Delta_{\text{HL}}(n) &= 2.4 + 4.3n^{-1}. \end{aligned} \quad (2)$$

As evident from Figure 2, as the number of layers n increases, E_b becomes larger, reaching the “infinite” polyprismane $E_b(\infty) = 4.9$ eV/atom. On the other hand, Δ_{HL} decreases, reaching $\Delta_{\text{HL}}(\infty) = 2.4$ eV. Similar dependencies are observed for $[n, 5]$ prismanes (see Figure 3).

Again E_b and Δ_{HL} depend linearly on n^{-1} (again, we do not take into consideration point with $n = 2$, which

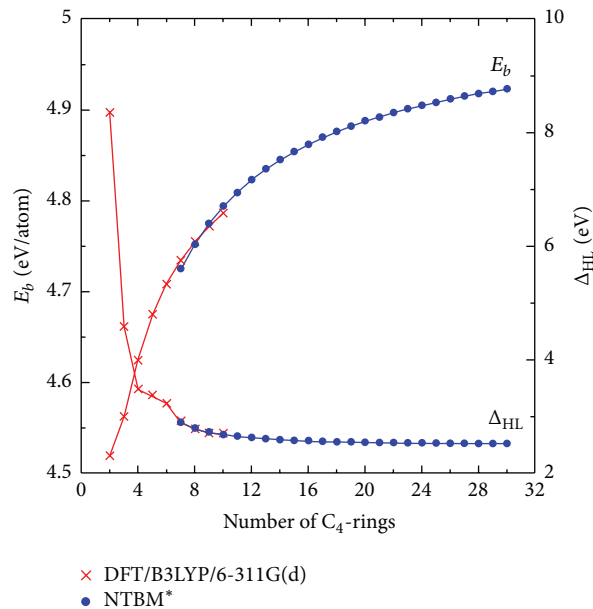


FIGURE 2: Binding energies and HOMO-LUMO gaps versus the number of C_4 -rings obtained at the DFT/B3LYP/6-311G(d) (crosses) and NTBM (circles) levels of theory. The asterisk indicates that all HOMO-LUMO gaps obtained within the NTBM model are shifted to 0.35 eV.

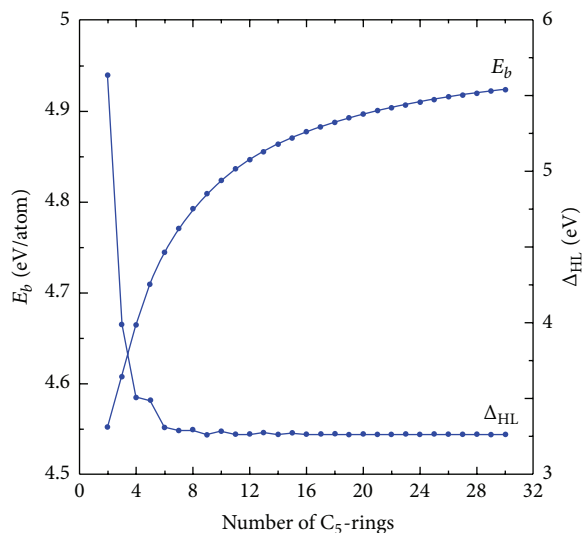


FIGURE 3: Binding energies and HOMO-LUMO gaps versus the number of C_5 -rings obtained within the NTBM model. All HOMO-LUMO gaps obtained are shifted to 0.35 eV.

corresponds to the pentaprismane $\text{C}_{10}\text{H}_{10}$ molecule). The analytic forms for $[n, 5]$ prismanes are

$$\begin{aligned} E_b(n) &= 4.9 - 0.9n^{-1}, \\ \Delta_{\text{HL}}(n) &= 3.2 + 1.8n^{-1}. \end{aligned} \quad (3)$$

The increase of E_b indicates that the $[n, 4]$ - and $[n, 5]$ prismanes become more thermodynamically stable as their effective lengths increase. In our opinion, the high

thermodynamic stability of “long” PP is associated with the decreasing of boundary induced structural distortions as the number of layers increases. As for HOMO-LUMO gap, such behavior is typical for low-dimensional carbon nanostructures, for example, carbon nanotubes [37], graphene nanoribbons [38], and carbon nanoflakes [39]. Note that Δ_{HL} values for “infinite” PP are near to the upper limit of characteristic semiconducting value. In other words, these values are comparable with the corresponding band gaps for the wide-bandgap semiconductors, such as GaP (2.3 eV), GaN (3.4 eV), and ZnSe (2.7 eV) [40]. So, in the bulk limit for pristine PP, it is not possible to transport electrons, but additional doping or mechanical stresses may induce charge transfer.

4. Conclusions

In this paper we presented structural, energy, and some electronic properties of $[n,4]$ - and $[n,5]$ prismanes with $n = 2 \div 30$. The data of numerical simulation obtained in this study indicate an increase of thermodynamic stability of PP as the number of layers n increases. Binding energies estimated for both “infinite” tetra- and pentaprismanes are equal to 4.9 eV/atom. In contrast to binding energies, HOMO-LUMO gaps decrease as the effective length of PP increases. In the bulk limit ($n \rightarrow \infty$) Δ_{HL} is equal to 2.4 and 3.2 eV for $[n,4]$ - and $[n,5]$ prismanes, respectively. These values are near to the upper limit of characteristic semiconducting value; therefore, it becomes possible to tune electronic properties of the PP by doping or mechanical stresses that will be useful for nanoelectronic applications.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

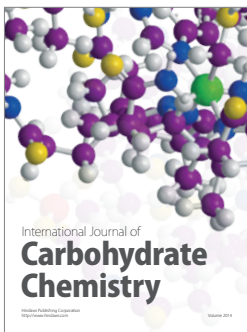
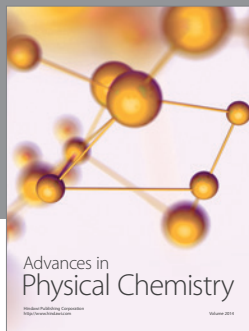
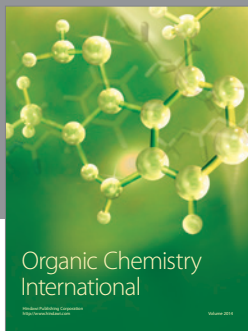
Acknowledgments

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