

Article

Bilayer C₆₀ Polymer/h-BN Heterostructures: A DFT Study of Electronic and Optic Properties

Leonid A. Chernozatonskii ^{1,2,*} and Aleksey I. Kochaev ^{3,4,*} 
¹ Emanuel Institute of Biochemical Physics RAS, 4 Kosygin Street, 119334 Moscow, Russia

² Scientific School on Chemistry and Technology of Polymer Materials, Plekhanov Russian University of Economics, 117997 Moscow, Russia

³ Research and Education Center “Silicon and Carbon Nanotechnologies”, Ulyanovsk State University, 42 Leo Tolstoy Street, 432017 Ulyanovsk, Russia

⁴ Laboratory of 2D Nanomaterials in Electronics, Photonics and Spintronics, National Research Nuclear University “MEPhI”, 31 Kashirskoe sh., 115409 Moscow, Russia

* Correspondence: chernol-43@mail.ru (L.A.C.); a.kochaev@ulsu.ru (A.I.K.)

Abstract: Interest in fullerene-based polymer structures has renewed due to the development of synthesis technologies using thin C₆₀ polymers. Fullerene networks are good semiconductors. In this paper, heterostructure complexes composed of C₆₀ polymer networks on atomically thin dielectric substrates are modeled. Small tensile and compressive deformations make it possible to ensure appropriate placement of monolayer boron nitride with fullerene networks. The choice of a piezoelectric boron nitride substrate was dictated by interest in their applicability in mechanoelectric, photoelectric, and electro-optical devices with the ability to control their properties. The results we obtained show that C₆₀ polymer/h-BN heterostructures are stable compounds. The van der Waals interaction that arises between them affects their electronic and optical properties.

Keywords: fullerenes; bilayers; boron nitride; graphene; van der Waals heterostructures; DFT



Citation: Chernozatonskii, L.A.; Kochaev, A.I. Bilayer C₆₀ Polymer/h-BN Heterostructures: A DFT Study of Electronic and Optic Properties. *Polymers* **2024**, *16*, 1580. <https://doi.org/10.3390/polym16111580>

Academic Editor: Joan Josep Cerdà

Received: 23 April 2024

Revised: 30 May 2024

Accepted: 31 May 2024

Published: 3 June 2024



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1. Introduction

Recent advances in nanoelectronics, hydrogen energy, and biotechnology are closely related to new nanoscale materials and structures with unique physical properties. Examples of such objects are fullerenes [1–3]. These carbon macromolecules, in particular C₆₀ fullerene, are used in nonlinear optics, semiconductor technology, electric batteries, pharmacology, the chemical industry, and biomedical technologies [4]. The discovery of the synthesis of monolayer C₆₀ polymers has returned interest in fullerene polymer structures [5]. They have been shown to be good semiconductors with anisotropic optical properties. Quantum chemical modeling confirms the stability of polymerized fullerenes and proves that they have interesting anisotropic optical, mechanical, and thermoelectric characteristics [6]. A high degree of hydrogen adsorption of fullerene layers placed on a graphene substrate is also shown [7].

At the same time, dielectric substrates are of great importance in nanoengineering. The most famous and easily reproducible is a substrate made of single or multilayer boron nitride [8]. As far as we know, there has been no study of the placement of fullerenes on a single-layer boron nitride substrate, nor has there been a study of sandwiched polymerized fullerenes between two layers of boron nitride. In this paper, we fill these gaps by focusing on the structural, electronic, and optical properties of heterostructures formed by polymerized fullerenes and boron nitride layers. We considered two types of structures, taking into account the stability of polymer monolayers, namely the quasi-hexagonal fullerene phase qhPC₆₀, in which each fullerene is bonded to its neighbors through four single and two cycloaddition bonds [2 + 2], and the hexagonal fullerene phase hPC₆₀, which is close to

the qhPC₆₀ structure in atomic structure (the 2D-18 polymer in the B. Mortazavi designation [9]), where the C₆₀ molecule is bonded by six [2 + 2] bonds to its neighbors—a model previously considered one of the pressure-induced C₆₀ polymers [10].

The stability of the considered fullerene networks is achievable by doping with magnesium and potassium [11]. It is expected that fullerene networks in heterostructures will be more stable [12–14]. In general, planar C₆₀ polymers are of great interest [15]. The combined use of C₆₀ polymer and *h*-BN monolayers has important practical benefits. Firstly, this heterostructure is a semiconductor material on a strong piezoelectric dielectric; therefore, it becomes possible to change the electronic spectrum (conductivity and optical response) using structural deformation and (or) doping with foreign atoms. These can be mechanical–electrical sensors that respond to the appearance of electrical voltage on the film or optically excited ones. Secondly, this hybrid material is easy to manufacture due to the currently well-studied components that make it up.

2. Computational Methods

Computational design and procedure were carried out using the Quantum ATK software 2021.06 [16]. Structural optimization and calculation of the main characteristics of heterostructures under consideration were performed using atomistic modeling based on density functional theory (DFT) in the linear combination of atomic orbitals (LCAOs) approximation. The generalized gradient approximation (GGA) for the exchange and correlation potential expressed by the Perdew–Burke–Ernzerhof (PBE) functional and the projector augmented-wave potential (PAW) are used to obtain equilibrium atomic configurations of the heterostructures [17]. To obtain the electronic spectra, the Heyd–Scuseria–Ernzerhof hybrid exchange–correlation functional is applied [18]. All calculations were carried out using periodic boundary conditions. To neglect the influence of the periodic images in the *z*-direction perpendicular to the sheet, we take the value of the cell parameter along *z* equal to 15 Å. The van der Waals interaction was taken into account using the DFT-D2 method of Grimme [19]. The use of these approaches has previously made it possible to predict entire families of two-dimensional materials [20].

The projected density of states (PDOSs) is the relative contribution of a particular atom (or orbital) to the total density of states. Associated with a given projection *M*, the PDOS is defined as

$$D_M(\epsilon) = \sum_n \delta(\epsilon - \epsilon_n) \langle \varphi_n | \widehat{P}_M | \varphi_n \rangle, \quad (1)$$

where φ_n are the eigenstates, $|\widehat{P}_M|$ is a projection operator [21], and *n* includes all the quantum numbers of the system.

The optical properties were characterized by the absorption coefficient α_a . Its calculation is based on solving a system consisting of the Kubo–Greenwood equation for the components of the susceptibility tensor χ_{ij} [22]

$$\chi_{ij}(\omega) = -\frac{e^2 \hbar^4}{m^2 \epsilon_0 V \omega^2} \sum_{nm} \frac{f(E_m) - f(E_n)}{E_{nm} - \hbar\omega - i\Gamma} \pi_{nm}^i \pi_{nm}^j, \quad (2)$$

and the coupling equations

$$\begin{aligned} n + i\kappa &= \sqrt{\epsilon_r}, \\ \epsilon_r(\omega) &= (1 + \chi(\omega)), \\ \alpha_a &= 2 \frac{\omega}{c} \kappa, \end{aligned} \quad (3)$$

where *V* is a volume of the considered cell, ω is a electromagnetic wave frequency, *f* is the Fermi–Dirac function, $\Gamma = 0.1$ eV is the broadening, π_{nm}^i is the *i*-th dipole matrix element between the states *m*' and *m*, *n* is the refractive index, κ is the extinction coefficient, ϵ_r is the relative dielectric constant, and *c* is the speed of light.

To clearly see the redistribution of electrons on the components of the considered heterostructures, we study the electron localization function (ELF). The ELF is defined as [23].

$$\begin{aligned} \text{ELF} &= \frac{1}{1 + (D/D_h)^2}, \\ D &= \frac{1}{2} \sum_i |\nabla \varphi_i|^2 - \frac{1}{8} \frac{|\nabla \rho|^2}{\rho}, \\ D_h &= \frac{3}{10} (3\pi^2)^{2/3} \rho^{5/3}, \end{aligned} \quad (4)$$

where φ is the Kohn–Sham orbital, and ρ is the local density. The electron localization function, ranging from 0 to 1, takes the value 0 if there are regions of space where the electrons are perfectly delocalized, and it takes a value of 1 if high electron localization can be observed.

3. Results and Discussion

3.1. Geometric Structures and Properties of Individual Units

Ways for incorporating C_{60} and other fullerene molecules into polymer structures are described in detail in [9,24]. We limited ourselves to the hexagonal (HPC_{60}) and quasi-hexagonal fullerene phases (qHPC_{60}). The two considered types are stable. The presented fullerene sets are held covalent bonds. To calculate the binding energy acting between individual C_{60} molecules in polymerized fullerene sets, we use the following expression

$$E_b = E_{\text{HPC}_{60}/\text{qHPC}_{60}} - E_{C_{60}} \quad (5)$$

where $E_{\text{HPC}_{60}/\text{qHPC}_{60}}$ is the total energy of cells containing the atomic configuration of one polymerized fullerene phase, $E_{C_{60}}$ is the same, but for a free fullerene molecule. The same energies for both HPC_{60} and qHPC_{60} fullerene phases are -1.372 eV and -1.281 eV, respectively. In the hPC_{60} fullerene phase, the C_{60} molecule is bonded by six bonds to its neighbors. In the qhPC_{60} phase, each fullerene is bonded to its neighbors through four single and two cycloaddition bonds. The atomic configurations and unit cells of optimized monolayer boron nitride and two polymerized sets of fullerenes in the HPC_{60} and qHPC_{60} form are depicted in Figure 1.

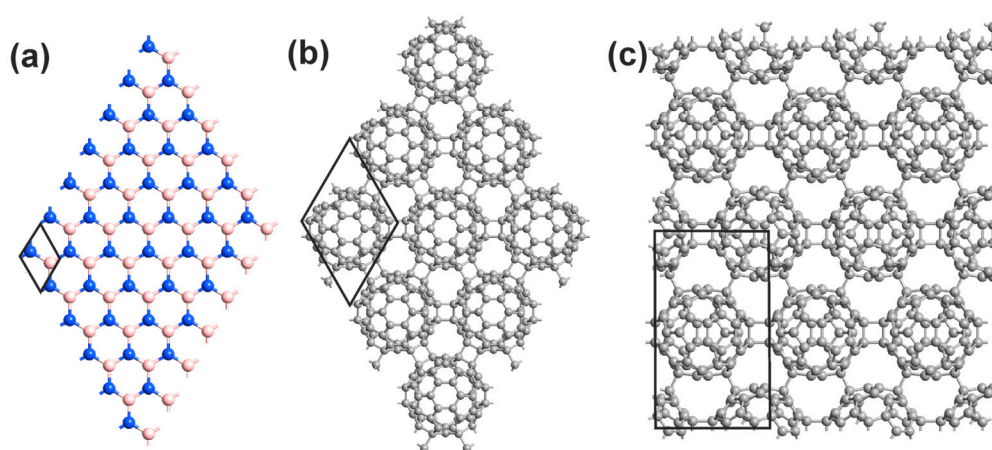


Figure 1. Atomic configurations and unit cells of optimized monolayer boron nitride (a) and two polymerized sets of fullerenes (b,c). Blue, pale pink, and grey colors denote the nitrogen, boron, and grey atoms. Black lines highlight the unit cells of the heterostructures. Lattice parameter is $2.50 \text{ \AA}$ for monolayer boron nitride; $9.21 \text{ \AA}$ for the HPC_{60} fullerene phase; and $15.8 \text{ \AA}$ and $9.17 \text{ \AA}$ for the qHPC_{60} fullerene phase.

Figure 1 shows relaxed atomic configurations and unit cells independent of each other, obtained in the course of solving the problem of optimization of geometric and energy parameters. In order to further compare the electronic and optical spectra of the assemblies and solitary layers, we present the results of calculations of electronic band structures (EBSs), densities of electronic states (DOSs), and optical absorption spectra (OAS) for all three layers separately. Figure 2 shows the EBS, DOS, and OAS of monolayer boron nitride, HPC₆₀ fullerene phase, and qHPC₆₀ fullerene phase. The characteristic values correspond to the DFT-HSE calculation scheme.

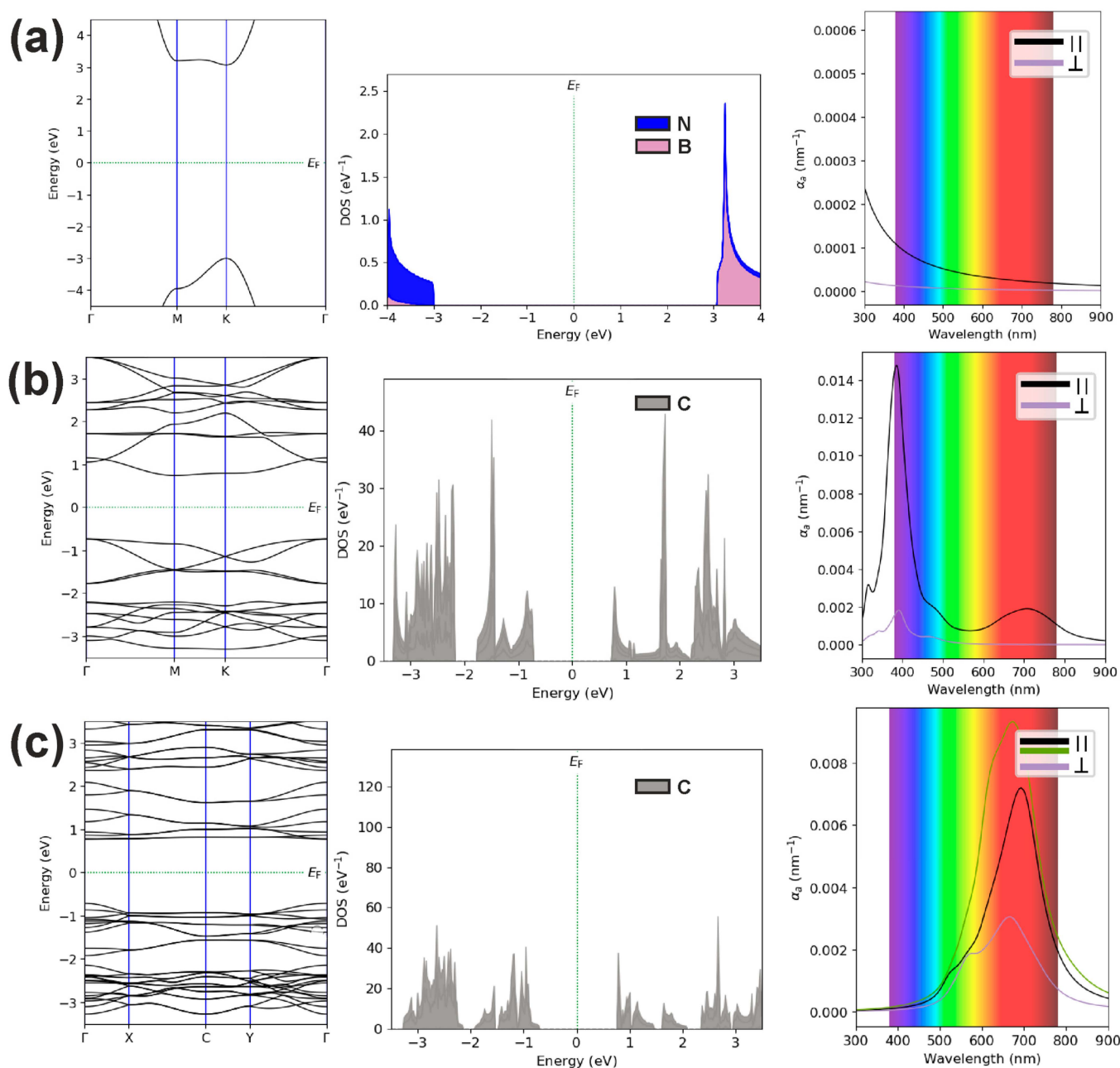


Figure 2. The electronic band structures, densities of electronic states, and optical absorption spectra of monolayer boron nitride (a), HPC₆₀ fullerene phase (b), and qHPC₆₀ fullerene phase (c).

3.2. Geometric Structures and Properties of Heterostructures

An atomistic modeling approach makes it possible to easily construct nanoscale complexes from different materials into single assemblies and to draw reliable conclusions about the feasibility of synthesis. Moreover, these methods help to investigate the physicochem-

ical properties and characteristics of predicted materials and structures. We constructed cells containing heterostructures of the “C₆₀ polymer/*h*-BN” type, where fullerene HPC₆₀ and qHPC₆₀ phases acted as the polymers. Atomic images of these relaxed heterostructures are shown in Figure 3.

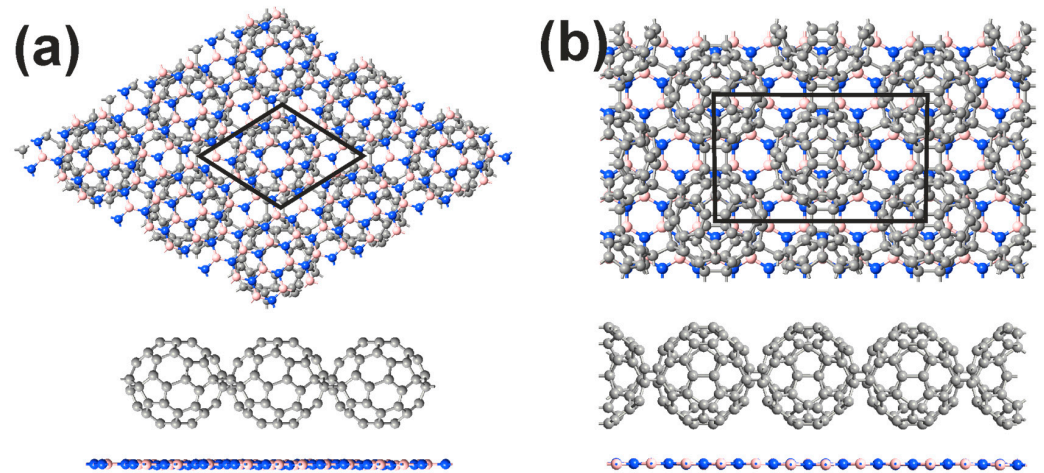


Figure 3. The atomic configurations and unit cells of optimized C₆₀ polymer/*h*-BN heterostructures formed from monolayer boron nitride and HPC₆₀ phase of polymerized fullerene (a) and monolayer boron nitride and qHPC₆₀ phase of polymerized fullerene (b). Black lines highlight the unit cells of the heterostructures. Lattice parameter is 9.13 Å for the C₆₀ (HPC₆₀)/*h*-BN heterostructure; 15.4 Å and 8.91 Å for the C₆₀ (qHPC₆₀)/*h*-BN heterostructure.

In the bilayer heterostructures under consideration, the lattices of the monolayer *h*-BN and both polymerized fullerene sets are incommensurate. For each case, we simulated a general “try-in” superlattice on the *h*-BN layer so that when superimposed on a C₆₀ polymer unit cell, it would produce the closest commensurate configuration for the selected heterostructure. This is also performed when vertically assembling two different hexagonal layers of graphene and boron nitride. Since the C₆₀ (HPC₆₀)/*h*-BN heterostructure consists of two hexagonal atomic layers, by rotating one layer relative to the other, one can obtain a commensurate structural version with the lowest lattice mismatch. How to determine the twisting angle is shown in [25,26]. Using it, we found the most acceptable option with a small number of atoms in the supercell containing one fullerene and a rotated boron nitride layer with a rotated angle of 13.9°. The choice of the supercell in the case of the C₆₀ (qHPC₆₀)/*h*-BN heterostructure was carried out by selecting a rectangular boron nitride supercell, which was closest to the unit cell of the polymer C₆₀ qHPC₆₀ layer.

After DFT-PBE optimization, no strong distortions occurred in both the *h*-BN or polymerized C₆₀ layers. As shown in Figure 3, no covalent bonds form between *h*-BN and HPC₆₀ (qHPC₆₀) fullerene phase. Apparently, the hetero-assembly is maintained due to van der Waals forces. The resulting (optimal) distance between the qHPC₆₀ fullerene phase and *h*-BN is smaller compared to that of the C₆₀ (HPC₆₀)/*h*-BN heterostructure (3.03 Å vs. 3.25 Å). Accordingly, the bonding between *h*-BN and qHPC₆₀ should be somewhat stronger. Let us check this by calculating the binding energy E_b using the formula

$$E_b = E_{hetero} - (E_{h-BN} + E_{HPC60/qHPC60}) \quad (6)$$

and take structural units (the monolayer and the set of same fullerenes in the polymerized form) as reference systems. Here, E_{hetero} is the total energy of the cell containing the atomic configuration of the heterostructure composed of the polymerized fullerene phase and a substrate from a single-layer boron nitride; E_{h-BN} , $E_{HPC60/qHPC60}$ are the same, but for a free fullerene molecule and the polymerized fullerene phase, respectively. The binding energy of the C₆₀ (qHPC₆₀)/*h*-BN heterostructure is equal to −0.529 eV, while the binding energy of

the C_{60} (HPC₆₀)/*h*-BN heterostructure is -1.069 eV. Apparently, direct comparison between the bonding strength and interlayer distance is impossible in this case. The fullerene sets and *h*-BN are deformed differently in the resulting heterostructures. Values of the same B–N and C–C bond length in both individual species and corresponding heterostructures are presented in Table 1. As shown in Table 1, in both heterostructures, the B–N bonds are stretched. This stretching occurs due to the weak compressibility of fullerenes. The lengths of interfullerene bonds decrease more (1.59 Å vs. 1.55 Å) than other C–C bonds. In order to fit two structures into a single assembly and reduce mismatching, the weakest bonds will deform most easily. Apparently, it is interfullerene bonds that are such.

Table 1. Values of same bond length (Å) of the individual species and corresponding heterostructures. The values correspond to relaxed configurations. Selected bond lengths (A, D, C, and D) are presented in Figure S1 in Supplementary Materials. Interfullerene bonds are highlighted in bold.

Bond Type	<i>h</i> -BN	HPC ₆₀ Fullerene	qHPC ₆₀ Fullerene	C_{60} (HPC ₆₀)/ <i>h</i> -BN	C_{60} (qHPC ₆₀)/ <i>h</i> -BN
B–N	1.45			1.46	1.48
C–C		1.36 (A)	1.41 (A)	1.36	1.41
		1.40 (B)	1.45 (B)	1.39	1.45
		1.52 (C)	1.48 (C)	1.51	1.50
		1.59 (D)	1.59 (D)	1.58	1.55

Figure 4 shows the EBS, DOS, and OAS of C_{60} polymer/*h*-BN heterostructures, where fullerene HPC₆₀ and qHPC₆₀ phases acted as the polymer. As follows from the Figure 4, their spectra differ from the spectra of individual components of the heterostructures (Figure 2b,c). Moreover, Figure 4 indicates charge redistribution due to the presence of a boron nitride monolayer in the heterostructure. As follows from the calculated density of states, the states of nitrogen atoms make their contributions over a wide range of energies.

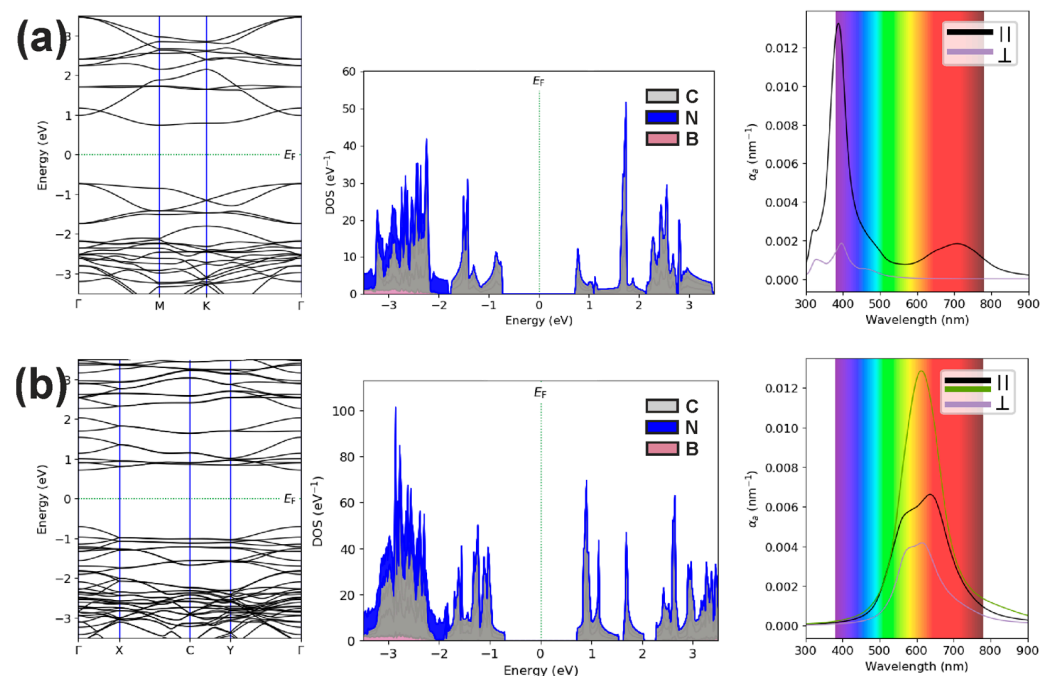


Figure 4. The electronic band structures, densities of electronic states, and optical absorption spectra of C_{60} polymer/*h*-BN heterostructures, where fullerene HPC₆₀ (a) and qHPC₆₀ (b) phases acted as the polymer.

In the C_{60} (qHPC₆₀)/*h*-BN heterostructure, small charge transfer occurs between the components with a redistribution of the electron density in them, which leads to a decrease

in the band gap to 1.42 eV from 1.48 eV compared to the free fullerene qHPC₆₀ phase. For the fullerene HPC₆₀ phase, this difference is smaller: 0.02 eV. The ability to easily stretch the presented polymerized fullerenes greatly influenced the value of the band gap we obtained when using one or another atomistic calculation model. In this regard, the band gaps and light absorptions we obtained differed (by 5% and high transformation) from those listed in [5,6]. A summary of the calculated data on the structural and electronic properties of the considered heterostructures and individual layers is presented in Table 2. In the 3rd and 4th columns, the binding energies correspond to the formation of the sets from single fullerenes, but in the 5th and 6th columns, the binding energies correspond to the formation of the heterostructures.

Table 2. Values of lattice parameter d , binding energy E_b , and band gap E_g of the individual species and corresponding heterostructures.

	<i>h</i> -BN	HPC ₆₀ Fullerene	qHPC ₆₀ Fullerene	C ₆₀ (HPC ₆₀)/ <i>h</i> -BN	C ₆₀ (qHPC ₆₀)/ <i>h</i> -BN
d , Å	2.50	9.21	15.8; 9.17	9.13	15.4; 8.91
E_b , eV		−1.372	−1.281	−1.069	−0.529
E_g , eV	6.08	1.48	1.48	1.47	1.42

The calculated optical absorption coefficients for components parallel and perpendicular to the heterostructure plane show strong anisotropic behavior, just as in the case of free C₆₀ polymers. As can be seen, when using a monolayer boron nitride substrate for the HPC₆₀ fullerene phase, the optical absorption is slightly weakened (0.0145 vs. 0.0132 nm^{−1}), while for the qHPC₆₀ fullerene phase, on the contrary, it increases (0.0128 vs. 0.0093 nm^{−1}) and spectra change. In the obtained electronic spectra, strongly flattened minibands are visible near the conduction band minima and the valence band maxima, giving high DOS values at a number of certain energies. This indicates the possibility of observing resonant optical, nonlinear optical, and photoelectronic properties in the proposed heterostructures. Since the heterostructures considered do not have a center of symmetry and, therefore, are piezoelectric and non-linear optical media, they can be used to create new planar devices that use their nonlinear optical [27] and acoustoelectric [28] properties.

Figure 5 shows the ELF values projected and summarized in a line along the z -direction of the constructed cells. Since the line “accumulates” all contributions along the preferred direction, the localization of electrons between the boron nitride monolayer and fullerene sets can be determined by the numerical value. The integrated ELF between both the fullerene sets and boron nitride monolayer does not exceed 0.1, which is very small.

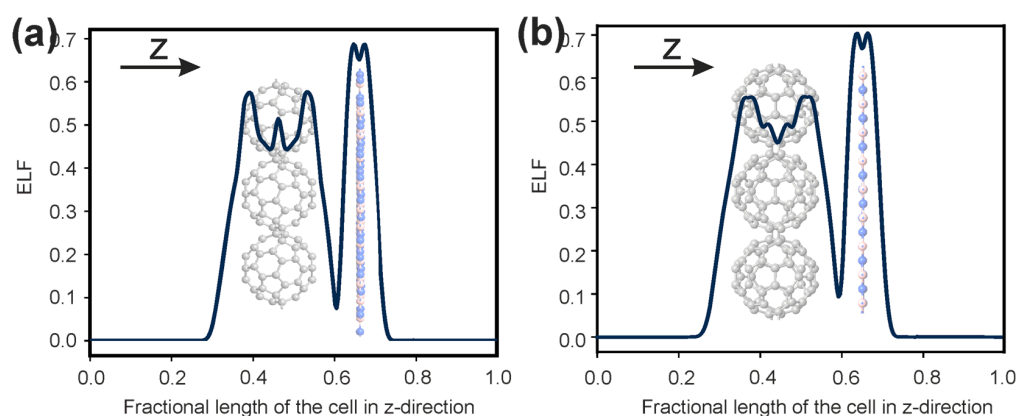


Figure 5. The ELF values projected onto line along z -direction of the constructed cells: (a) the case of C₆₀ (HPC₆₀)/*h*-BN heterostructure; (b) the case of C₆₀ (qHPC₆₀)/*h*-BN heterostructure.

4. Conclusions

In this study, we focused on the interaction of a boron nitride monolayer with polymerized fullerene molecules. The effect of interaction between a boron nitride substrate and a network of fullerenes, which is missing in the literature, was considered. The emerging van der Waals interaction, in some cases, changes the electronic and optical spectra. The calculated formation energies show that the deposition of fullerenes onto a single-layer boron nitride substrate is advantageous. The resulting heterostructure must be stable. Using the monolayer boron nitride dielectric substrate to support the presented fullerene sets is a good way to preserve their semiconducting properties. The choice of piezoelectric boron nitride substrate was dictated by interest in the considered van der Waals bilayers in mechanoelectric, photoelectric, and electro-optical device applicability with the ability to control their properties.

Supplementary Materials: The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/polym16111580/s1>, Figure S1: Selected bond lengths for analysis of tuning of fullerene sets in the C₆₀ polymer/h-BN heterostructures (left—HPC₆₀ fullerene set, right—qHPC₆₀ fullerene set).

Author Contributions: Conceptualization, L.A.C.; methodology and modelling, L.A.C.; software, A.I.K.; validation, L.A.C. and A.I.K.; investigation, A.I.K.; resources, L.A.C.; data curation, A.I.K.; writing—original draft preparation, L.A.C.; writing—review and editing, L.A.C. and A.I.K.; visualization, L.A.C. and A.I.K.; project administration, L.A.C.; All authors have read and agreed to the published version of the manuscript.

Funding: The work was partially carried out within the framework of the project (No. 122041400110-4) of the federal budget of the Russian Ministry of Science and Higher Education. The work was partially supported by the Ministry of Science and Higher Education of the Russian Federation, project FSWU-2024-0014.

Institutional Review Board Statement: Not applicable.

Data Availability Statement: Data are contained within the article.

Conflicts of Interest: The authors declare no conflicts of interest.

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