Review
Nanostructured, nanoscale materials and nanodevices

УДК 538.9 DOI: 10.17277/jamt-2026-11-02-194-204

Modified carbon nanotubes in polymethylmethacrylate and polypropylene matrices: DFT modeling of electronic energy structure, creation technologies and application prospects (review)

© Lusine S. Elbakyan[a]✉

[a] *Volgograd State University, 100, Universitetskiy Av., Volgograd, 400062, Russian Federation*

✉ lusniak-e@yandex.ru

Abstract. This article presents a review of contemporary studies on the production of composite materials based on polymethyl methacrylate (PMMA) and polypropylene (PP) with improved properties. The formation of a coherent scientific understanding of the processes involved in producing nanocomposites underpins the development of next-generation materials. In such systems, conventional polymers serve as the matrix, while carbon nanotubes act as the conductive filler. The study of effects that arise from the introduction of ultra-small quantities of carbon nanoparticles is of key importance here: it is precisely these effects that enable a dramatic change in a wide range of polymer properties without significantly increasing material costs. Alongside experiments aimed at improving conductive polymers, multiscale modeling is playing an increasingly priority role. Computational experiments reduce development costs and predict the stability of materials under load, transforming modeling into a key driver of technological progress in the field of organic electronics. Confirming the effectiveness of computational methods, the authors of this article present the findings of their own research on the interaction mechanisms between the aforementioned polymers and single- and double-walled carbon nanotubes, which led to the creation of a composite polymer system. This research was conducted using a modern quantum-chemical method – density functional theory (DFT). Thus, the presented review not only summarizes existing achievements in the field of CNT/PMMA and CNT/PP composites, but also establishes a new methodological vector in which computational methods (particularly DFT) become an equal and, at early stages, a priority tool for designing nanocomposites with predictable properties.

Keywords: polymethylmethacrylate; polypropylene; carbon nanotubes; polymer nanocomposites; density functional theory; adsorption interaction; conductive properties.

For citation: Elbakyan LS. Modified carbon nanotubes in polymethylmethacrylate and polypropylene matrices: DFT modeling of electronic energy structure, creation technologies and application prospects (review). *Journal of Advanced Materials and Technologies*. 2026;11(2):194-204. DOI: 10.17277/jamt-2026-11-02-194-204

Модифицированные углеродные нанотрубки в матрицах полиметилметакрилата и полипропилена: DFT-моделирование электронно-энергетической структуры, технологии создания и перспективы применения (обзор)

© Л. С. Элбакян[a]✉

[a] *Волгоградский государственный университет, пр. Университетский, 100, Волгоград, 400062, Российская Федерация*

✉ lusniak-e@yandex.ru

Аннотация. Статья содержит обзор современных работ, посвященных получению композиционных материалов на основе полиметилметакрилата (ПММА), полипропилена (ПП) с улучшенными характеристиками. Формирование целостных научных представлений о процессах получения нанокомпозитов лежит в основе создания материалов нового поколения. В таких системах матрицей служат традиционные полимеры, а функцию проводящего наполнителя выполняют углеродные нанотрубки. Ключевое значение здесь приобретает изучение эффектов, возникающих при введении сверхмалых количеств углеродных наночастиц: именно они позволяют кардинально изменить широкий спектр свойств полимеров без значительного удорожания материала. Наряду с экспериментами по улучшению проводящих полимеров все более приоритетную роль играет многомасштабное моделирование. Вычислительные эксперименты сокращают затраты на разработку и прогнозируют стабильность материалов при нагрузках, что превращает моделирование в ключевой драйвер технологического прогресса в области органической электроники. Подтверждая эффективность вычислительных методов, авторы приводят результаты собственных исследований механизмов взаимодействия перечисленных полимеров с одно- и двуслойными УНТ, приведших к созданию композитной полимерной системы, выполненных с использованием современного квантово-химического метода – теории функционала плотности DFT. Таким образом, представленный обзор не только обобщает существующие достижения в области композитов УНТ/ПММА и УНТ/ПП, но и задает новый методологический вектор, в котором вычислительные методы (в частности, DFT) становятся равноправным, а на начальных этапах – приоритетным инструментом проектирования нанокомпозитов с прогнозируемыми свойствами.

Ключевые слова: полиметилметакрилат; полипропилен; углеродные нанотрубки; полимерные нанокомпозиты; метод теории функционала плотности; адсорбционное взаимодействие; электропроводящие свойства.

Для цитирования: Elbakyan LS. Modified carbon nanotubes in polymethylmethacrylate and polypropylene matrices: DFT modeling of electronic energy structure, creation technologies and application prospects (review). *Journal of Advanced Materials and Technologies*. 2026;11(2):194-204. DOI: 10.17277/jamt-2026-11-02-194-204

1. Introduction

Over the past decades, interest in nanostructures based on conductive polymers has steadily increased in both fundamental science and applied industries. This field has seen particularly rapid development in the last ten years, driven by the discovery of unique properties in nanoscale forms of these materials and significant increases in the efficiency of devices based on them [1].

Market growth is driven by the automotive and diesel industries, as well as the general demand for lightweight, high-performance, and affordable electronic components. However, to reach the mass market, it is necessary to dramatically improve the processability of these polymers. The main challenges relate to their sensitivity to temperature and time fluctuations, as well as the nonlinear nature of their physicochemical properties.

The focus of modern research is on the creation of polymer composite materials reinforced with nanoscale fillers, including carbon nanotubes (CNTs) [2–6]. As evidenced by an analysis of the extensive scientific literature [7–9], CNTs occupy a key position in the field of composites due to their unique combination of thermal, mechanical, electrical, and optical properties. Growing interest in integrating CNTs into various polymer matrices is stimulating the development of CNT-based polymer nanocomposites, as well as hybrid polymer/fiber composites, which boast exceptional performance characteristics [10]. Advances in the technologies for producing such materials are considered among the most significant advances in nanoscience, as well as for biomedical, aerospace, construction, and other industries [11–15].

Along with in-depth experimental research aimed at improving the stability and processability of conductive polymers, the development of theoretical and computational foundations for their behavior under real-world operating conditions is of fundamental importance.

The development of multiscale modeling of conductive polymers will be able to link quantum-chemical calculations of binding energies, molecular dynamics descriptions of charge transfer, and continuum models of mechanical relaxation into a unified picture. Computational experiments should precede synthesis, minimizing development costs, and accompany production, allowing for the prediction of long-term material stability under cyclic loads and temperature fluctuations. This approach transforms modeling from an academic tool into a key driver of technological progress in organic electronics and “smart” materials.

A promising approach to assessing the effectiveness of nanofillers involves quantifying the interaction between the nanofiller and the polymer matrix by studying the electron-energy parameters of the process. This not only improves efficiency but also minimizes the need for practical testing. The quality of the adsorption interaction determines the stability of the resulting polymer-CNT complex. Given the difficulties associated with directly measuring the interaction energy of the studied complexes experimentally, computational methods offer a good alternative. Density functional theory calculations for solid-state systems yield results that are in good agreement with experimental data. Therefore, this method allows for studying the interaction between different types of nanofillers and polymers.

The aim of this study is to review modern approaches to producing polymethyl methacrylate and polypropylene-based composite materials with improved properties, as well as to develop and validate a computational approach (based on density functional theory (DFT)) for quantitatively assessing adsorption interactions in a polymer-carbon nanotube complex, ensuring the best balance between the accuracy of describing the electron-energy parameters and computational costs.

Determining the optimal functional and basis set for density functional theory calculations is a prerequisite for achieving computational reliability and depends on a number of factors, such as the purpose of the study, the size and complexity of the system, the type of interactions, computational resources, etc. For large systems (e.g., biomolecules or materials), a tradeoff between accuracy and computational costs may be required. Thus, the optimal choice of functional and basis set is a balance between the required accuracy and available computational resources.

We investigated the effectiveness of functionals in studying nanoparticles with semiconductor-like conductivity using GaAs quantum dots and 5CB (4-pentyl-4-cyanobiphenyl) liquid crystals [16]. Theoretical calculations showed that the B3LYP functional is the most preferable for such systems, as the obtained results are in good agreement with experimental results and theoretical calculations by other authors [17–19]. In [20], we tested the choice of functionals and basis sets for the quantum-mechanical DFT calculation method for TiO_2 nanotubes. There are also works by other authors in which the B3LYP functional in combination with the 3-21G basis set, known as B3LYP/3-21G, has demonstrated accurate results for a number of chemical systems, including complex organic molecules such as natural resins or polymers [21, 22].

2. PMMA-CNT polymer composite materials

Polymethyl methacrylate (PMMA) is a lightweight, non-toxic synthetic polymer with high transparency, weather resistance, and good physical, mechanical, and electrical insulating properties (Fig. 1). It is characterized by high impact strength, light transmittance, processability, and biocompatibility [23]. Due to this, PMMA is widely used in lighting engineering, medicine, aviation, and mechanical engineering. However, its thermal and mechanical stability are insufficient to meet modern industrial requirements, making modification of the material a pressing issue. The creation of new PMMA-based composites with predictable physical and mechanical properties will significantly expand its applications.

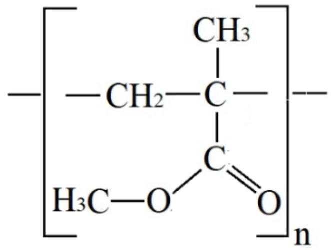

Fig. 1. The structural formula of polymethylmethacrylate

2.1. Experimental study of PMMA-CNT composite materials

The introduction of carbon nanotubes into polymer matrices plays a key role in expanding the potential application of composites, providing an increase in the elastic modulus and strength. To achieve the desired result, the method of producing the composite material plays a significant role. For example, in [24], using the 3D mixing method, various concentrations of multiwalled CNTs (MWCNTs) were introduced into PMMA to create polymer nanocomposites, followed by injection molding. Properties such as permittivity, conductivity, dielectric loss tangent, and electric modulus at intermediate frequencies were studied. The authors state that the findings have significant potential for application in electronics, sensors, and advanced materials, which emphasizes the novelty and practical significance of the study.

In [25], PMMA/MWCNT composites with concentrations of 2.5, 5, and 10 wt. % were obtained by mixing solutions. It was found that at 5 wt. % with the addition of 5 wt. % MWCNTs, the elastic modulus and hardness increase by 44 and 27 %, respectively, relative to pure PMMA. A further increase in the nanotube content to 10 wt. % leads to a decrease in these parameters by 23 and 28 %, respectively, compared to the sample containing 5 wt.%. Dynamic mechanical analysis in the frequency range of 50–210 Hz showed that the composite with 5 wt. % MWCNTs outperforms pure PMMA in elastic modulus across the entire studied range. Thus, the authors of [24] confirmed the feasibility of using low MWCNT concentrations in PMMA composites for operation under low- and medium-frequency loads.

Studies [26, 27] have shown that an increase in the CNT content leads to an increase in the elastic modulus and a decrease in fracture strain. In [28], the effect of process parameters (pressure, holding time, melt temperature) and the CNT concentration on the mechanical properties of composites was studied using the injection molding method. It has been found that with an increase in the nanotube content from

0 to 1.5 wt. %, tensile strength and elongation at failure decrease by approximately 30 and 40 %, respectively, while hardness increases slightly.

A significant amount of research has been devoted to the development of highly effective PMMA/CNT-based materials for electromagnetic shielding [29, 30].

In [29], the absorption characteristics of electromagnetic radiation by PMMA/CNT nanocomposite foam with a laminated configuration were studied. The layered structure ensured an absorption band extension to 3.5 GHz (8.9–12.4 GHz), which is 0.8 GHz wider than that of a single-layer 2 mm thick foam, as well as a reduction in reflection losses over a wide frequency range. This was achieved by reducing reflectivity in the upper layer and increasing absorption in the lower layer.

In the review paper [31], various methods for synthesizing foamed carbon materials (3D printing, supercritical foaming, carbonization, etc.) were considered, and the electromagnetic interference shielding properties of polymer composites reinforced with CNTs were analyzed, including existing problems and prospects for their solution.

The optimization of structural solutions for improving absorption characteristics is of particular interest. In [32], a foam plastic design with alternating layers of pure PMMA and PMMA/CNTs, forming a gradient structure, was proposed. The absorption band was 3.2 GHz (8.8–12.0 GHz), and the minimum reflection loss reached − 30.2 dB at 8 wt. % CNTs.

In [33], the possibility of producing PMMA/CNT composite granules combining high electrical conductivity and optical transparency was demonstrated. Using the electrostatic assembly method, homogeneous decoration of PMMA particles with nanotubes was achieved at their content of only 0.0068–0.068 vol. %, which ensured the formation of conductive channels.

In [34], composites based on PMMA granules with a coating of MWCNTs dispersed in a thermoplastic polyurethane (TPU) matrix were studied as sensing elements for pressure measurements. As the load increases, the granules converge, forming three-dimensional conductive networks across the interphase boundaries, ensuring early contact even at low pressures. An additional advantage is the increased thermal conductivity of the material. The authors recommend these composites for use in pressure measurement systems. In [35], the possibility of controlling the electrical conductivity of PMMA/MWCNT nanocomposites through halogenation was demonstrated, enabling the formation of a stable percolation network and achieving high conductivity.

In [36], a technology for producing flexible monopole antennas from PMMA films filled with single-walled carbon nanotubes (SWCNTs) was presented. The characteristics (reflection coefficient, radiation patterns, and gain) were evaluated in the unbent and bent states, confirming the potential for using such films. In [37], rectangular and circular polymer antennas were developed in which carbon nanotubes completely replace copper in the conductive elements and grounding. The achieved balance between dimensions, gain and efficiency demonstrated the practical suitability of such designs.

2.2. Theoretical modeling of the PMMA-CNT composite system

The reviewed studies were devoted to the strengthening of a polymer matrix by carbon nanomaterials, as well as imparting conductive properties to it. A comparison of the mechanical properties before and after the introduction of the filler showed that carbon nanotubes are capable of reinforcing the matrix. Furthermore, it was established that their addition to a polymer dielectric can lead to the emergence of electrical conductivity. The contribution of researchers to the development of nanocomposites is outstanding. Nevertheless, the mechanisms of strengthening the same matrix by different types of nanotubes are of particular interest; this aspect requires further study. The DFT method has proven itself as one of the most accurate approaches for atomic analysis of the structure, stability, mechanical and electronic properties of new materials [38]. Modern DFT modeling also allows for the prediction of the characteristics of carbon nanocomposites [39]. In [40], extended tight binding (xTB), DFT, symmetry-adapted perturbation theory (SAPT), and molecular dynamics (MD) simulations were used to understand the interaction of PMMA polymer with industrial gases (H_2, O_2, N_2, and H_2O). A theoretical experiment allows us to investigate the behavior of gas molecules in the presence of PMMA, which is important for understanding their adsorption and solubility in the polymer matrix.

In [41], molecular dynamics was used to analyze the interaction of β-blockers with PMMA in a pure matrix and in water, providing reliable information on the potential role of PMMA at the molecular level in the environment when in contact with pharmaceutical pollutants.

In [42], theoretical modeling of PMMA composites with SWCNTs was performed.

The CNT diameters (0.54–1.08 nm), volume fractions (8.1–16.5 %), and temperatures (100–700 K) were studied. The results showed a significant improvement in mechanical properties at low SWCNT contents. Furthermore, double-walled carbon nanotubes (DWCNTs) were twice as strong as single-walled carbon nanotubes (DWCNTs) at the same simulation cell dimensions.

We conducted quantum-chemical modeling of the interaction of polymethyl methacrylate with carbon nanotubes of various types, diameters, and layer counts. Theoretical studies revealed the high sorption activity of polymethyl methacrylate with carbon nanotubes of varying layer counts. Figure 2 shows a model of the interaction between a PMMA fragment $[C_5H_8O_2]_{15}$ and DWCNTs. We also studied the electron-energy structure of polymer nanocomposites based on polymethyl methacrylate, an analysis of which revealed that the complexes in question are narrow-bandgap semiconductors [43–48].

In [49], the effect of boron (16–50 %) on the adsorption of methyl methacrylate by boron-carbon nanotubes was studied. Quantum-chemical calculations showed that boron modification increases the adsorption energy by 45–50 % compared to pure tubes due to donor-acceptor interactions and electron density redistribution. The stability of the complex is ensured by physical adsorption with a Coulomb contribution. Boron-carbon nanotubes (p-semiconductors) improve the electrical conductivity of the composite and its mechanical properties (strength, elastic modulus), which is promising for flexible electronics and sensors.

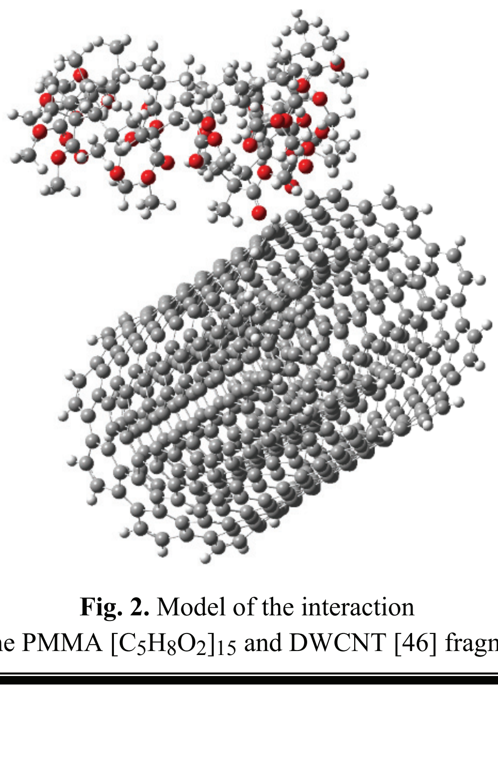

Fig. 2. Model of the interaction of the PMMA $[C_5H_8O_2]_{15}$ and DWCNT [46] fragment

The results obtained through quantum-chemical modeling are of direct practical significance, as they allow us to predict the effectiveness of using polymethyl methacrylate nanocomposites with carbon nanotubes as semiconductor materials for micro- and nanoelectronics. The theoretical data presented in this paper provide the basis for the targeted creation of such composites with tailored performance properties, promising for use in solar energy, microelectronics, optical materials, and polymer-based photoelectronic engineering.

3. Polypropylene-CNT polymer composite materials

Polypropylene is one of the most sought-after thermoplastics due to its high chemical resistance to acids, alkalis, and solvents, although it is unstable to non-polar liquids (Fig. 3). The material is characterized by low vapor permeability, good insulating properties, high air permeability, and water repellency. This explains its application in a variety of fields: from packaging and fibers to automotive, medical equipment, and household appliances.

Today, polypropylene is one of the most sought-after thermoplastics. This growth is driven by both increasing plastic consumption and improved processing technologies. However, the demands of modern industry are already exceeding the capabilities of traditional polymers [50].

The introduction of CNTs into a polymer matrix opens up the possibility of creating composites with improved electromagnetic shielding properties, which is relevant for electrical engineering, telecommunications, and the defense industry.

3.1. Experimental study of PP-CNT composite materials

The authors of [51] studied polypropylene composites reinforced with MWCNTs (0.4–1.5 wt. %), produced by compression molding. The introduction of MWCNTs increased the tensile strength to 62.80 % (at 1.2 wt. %), as well as the impact strength (by 82.14 %) and hardness (by 12.44 %) at the maximum filler concentration.

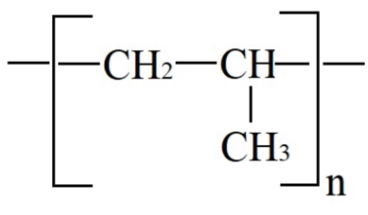

Fig. 3. Structural formula of the polypropylene molecule

In [52], it was shown that the addition of 5 wt. % carbon nanotubes to polypropylene improves the mechanical properties: the tensile strength increases by 11 %, Young's modulus by 33 %. Furthermore, the thermal stability of the composite increases by more than 30 °C compared to the original polymer.

The authors of [53] used microwave treatment to improve the mechanical properties of PP/MWCNT nanocomposites with a 10 % volume fraction of filler. This method promotes uniform volumetric hardening and increased strength. A strain rate sensitivity study showed that the tensile strength varied from 5.74 to 15.7 MPa depending on the loading rate. The highest flexural strength (21.91 MPa) and flexural modulus (2.69 GPa) were recorded at a rate of 1.25 $mm \cdot min^{-1}$. In [54], the effect of MWCNTs on the mechanical properties of polypropylene fiber concrete (PPFC) was studied. MWCNTs were dispersed in water using ultrasound and added in three dosages (0.05–0.15 % of the cement mass) with varying polypropylene fiber content (0.5–1.5 % of the mixture volume). The tests included compressive strength, flexural strength, tensile strength, elastic modulus, rebound number, and ultrasound velocity. Optimal results were obtained with 0.10 % MWCNTs and 1.0 % PPF: compression – 49.4 MPa, bending – 6.4 MPa, tension – 4.9 MPa, elastic modulus – 42257 MPa, rebound number – 47.0, ultrasound velocity – 5567 $m \cdot s^{-1}$. The addition of MWCNTs significantly improved the properties of PPFC, especially with this combination.

A number of studies [55, 56] are devoted to the study of creep and recovery of polypropylene with the introduction of carbon nanotubes. In [56], using coarse-grained MD modeling, it was shown that doping with CNTs increases the creep resistance of the nanocomposite. In [57], M. Sabet studied the effect of SWCNTs and MWCNTs on the thermal behavior and crystallization of isotactic polypropylene. It was found that the addition of nanotubes increases the crystallization temperature and the critical cooling rate without significantly changing the melting temperature. A percolation threshold of 0.5 wt. % was found for MWCNTs, at which the physical properties improved without the use of a compatibilizer. The increased interfacial surface area promotes increased thermal stability of the polymer, which opens up opportunities for the creation of high-performance nanocomposites based on PP. The authors of [58] also observed an improvement in the thermal stability of PP/CNT polymer composite materials.

The potential of using carbon nanotubes to impart high electrical conductivity to materials has long been confirmed [59–62]. Researchers worldwide are particularly interested in the development of conductive polymers and studying the potential for their practical use. In recent years, such polymers have found application in the creation of electronic devices, batteries, artificial muscles, solar energy conversion systems, and various types of sensors [63, 64].

In [65], it was shown that with an increase in the MWCNT content, the electrical conductivity of PP/MWCNT composites changes from insulating to semiconducting. Up to 3 wt. % of the material is non-conductive, but when this threshold is exceeded, a conductive network forms, and the conductivity increases sharply from 10^{-12} to 10^{-1} $S \cdot m^{-1}$, which corresponds to a percolation transition. Moreover, the conductivity is independent of the injection molding temperature.

In [66], statistical percolation theory methods were used to establish the electrical percolation threshold for PP/SWCNT composites at 1.4 wt. % (critical value $t = 2.05$). An optimized melt mixing process enabled the formation of a conductive network with an SWCNT content of approximately 1.28 wt. %. However, given the superior properties of SWCNTs compared to MWCNTs, such a low percolation threshold may not meet expectations.

In a number of studies [67–69], special nanocomposite production modes are used in addition to the introduction of CNTs to achieve conductive properties in polymeric materials. In [68], the effect of injection molding parameters on the crystalline structure and electrical resistance of PP/MWCNT composites was studied. The materials were produced by twin-screw melt extrusion followed by injection molding. With the same MWCNT content, increasing the mold temperature and injection speed resulted in a decrease in specific electrical resistance.

3.2. Theoretical modeling of the PP-CNT composite system

In parallel with the experimental work, a number of theoretical studies were conducted to explore the potential for improving the properties of polypropylene. In [70], the construction of seven models of PP-based composite materials was presented, and molecular dynamics (MD) simulations were conducted to determine the thermodynamic properties of these composite models. This study aimed to elucidate the microstructural mechanisms underlying the improved mechanical properties observed in functionalized MWCNT/PP composites. Furthermore, the study compared the effects of grafting different numbers of functional groups on improving the mechanical properties of PP composites.

Molecular models of CNT/PP nanocomposites containing randomly dispersed bundles of carbon nanotubes were also investigated in [71]. The modeling results showed that the properties of the modeled nanocomposite continuously improve with increasing nanotube content due to the effective CNT/PP interphase boundary and the reinforcing effect of the CNTs themselves.

In [72, 73] theoretical studies of the interaction processes of polypropylene (PP) polymer with carbon nanotubes of various types, diameters and layer density are presented. The adsorption process of one monomer unit (C_3H_6) of polypropylene, as well as a PP fragment [–$CH_2CH(CH_3)$–]$_n$ consisting of 15 structural units, was modeled. The E_{ad} values revealed the fact of physical adsorption of the polymer fragment with the CNT cluster. Thus, our results allowed us to predict the possibility of creating stable complexes of a composite polymer material based on nanotube-reinforced polypropylene. In this case, the adsorption energy value is fundamentally independent of the CNT layer density. We also analyzed the electron-energy structure of complexes formed by SWCNTs and DWCNTs and a polypropylene fragment [74]. The analysis of the band gap width ΔE_g of the complexes revealed that the system has a semiconductor conductivity type (Figs. 4, 5).

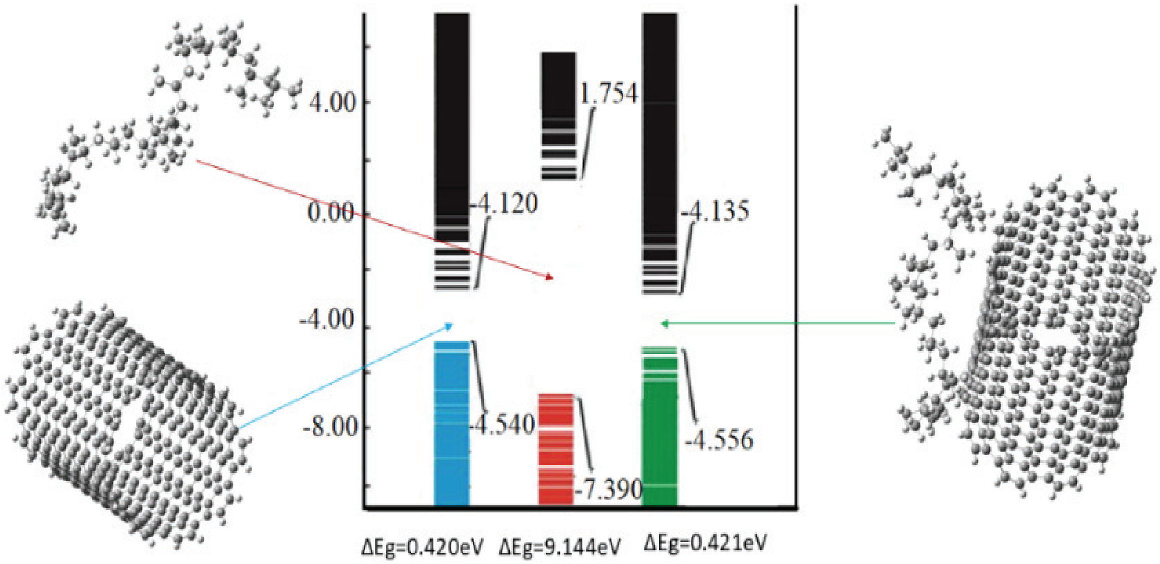

Fig. 4. Visualization of single-electron energy spectra of clusters of single-layer CNTs, a fragment of PP and interacting PP + CNTs modeling the structure of a composite polymer material [74]

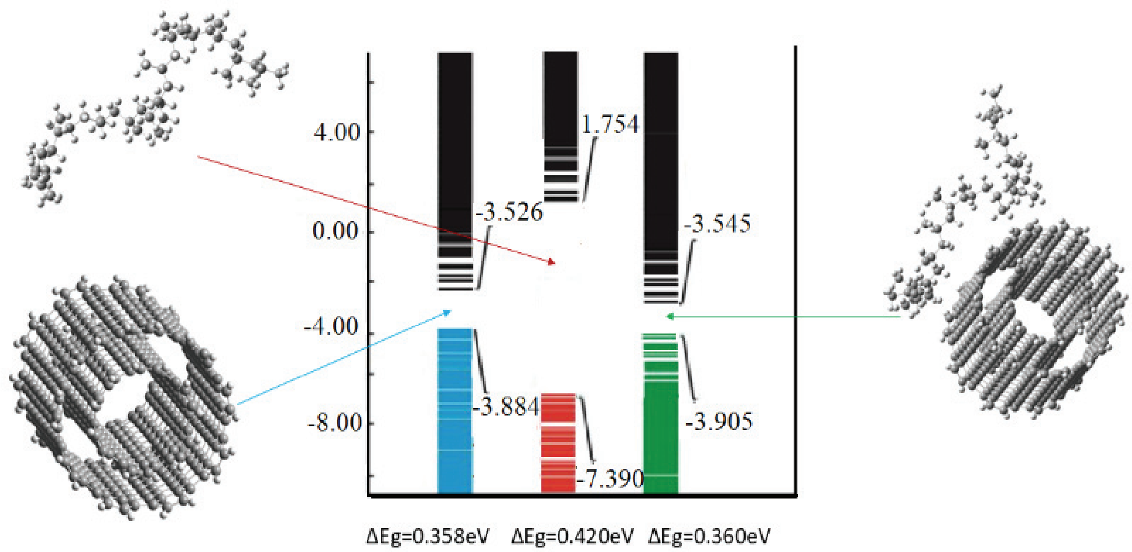

Fig. 5. Visualization of single-electron energy spectra of clusters of two-layer CNTs, a fragment of PP, and interacting PP + CNTs modeling the structure of a composite polymer material [74]

Thus, the introduction of the nanotubes under consideration into the polymer matrix of polypropylene, which is a dielectric by conductivity type, leads to the appearance of semiconducting properties in the resulting polymer nanocomposite.

4. Conclusion

The analysis of experimental studies on polymer composites based on polypropylene and polymethyl methacrylate with added carbon nanotubes demonstrates the wide range of applications for such materials. According to current data, PP/CNT and PMMA/CNT composites represent a promising area for further research and practical application. Improving production technologies opens up opportunities for creating new physical objects with both fundamental and applied significance. This review examines not only the unique physicochemical properties of polymers but also the effects arising from their modification with nanofillers. The composites obtained in this way exhibit enhanced mechanical, electrical, and radio-absorbing properties, opening up broad prospects for their application in various industries.

Ab initio calculations (DFT) reliably establish that the introduction of modified MWCNTs into PMMA and PP matrices leads to a restructuring of the electron-energy structure. Modifying carbon nanotubes in a polypropylene and polymethyl methacrylate matrix creates additional energy levels in the polymer's band gap, facilitating more efficient charge transfer at the interface.

Thus, the synthesis of DFT modeling data and fabrication technologies opens up prospects for creating polymer composites with tailored properties, defining a strategy for the further development of functional materials.

5. Funding

The present study did not receive any external funding.

Финансирование

Настоящее исследование не получило внешнего финансирования.

6. Conflict of interests

The authors declare no conflict of interest.

Конфликт интересов

Авторы заявляют об отсутствии конфликта интересов.

References

1. Mishra AK. Conducting polymers: concepts and applications. *Journal of Atomic, Molecular, Condensate and Nano Physics*. 2018;5(2):159-193. DOI:10.26713/jamcnp.v5i2.842

2. Shadrov SP, Butt HA, Vildanova AR, Agafonova EE, et al. Carbon nanotube fibers as high-fidelity sensors for carbon nanotube/polymer nanocomposites. *iScience*. 2026;29(4):115498. DOI:10.1016/j.isci.2026.115498

3. Ze Y, Liu Y, Wang B, Yin H, et al. Carbon nanotube materials for future integrated circuit applications. *Materials Today*. 2024;79:97-111. DOI:10.1016/j.mattod.2024.07.008

4. Malaya EV, Savvin AI. Composite materials in modern aviation. *Aktual'nye issledovaniya*. 2022;49(128):6-9. (In Russ.)

5. Chen J, Liu B, Gao X, Xu D. A review of the interfacial characteristics of polymer nanocomposites containing carbon nanotubes. *RSC Advances*. 2018;8(49):28048-28085. DOI:10.1039/C8RA04205E

6. Pour GB, Ashourifar H, Aval LF, Solaymani S. CNTs-supercapacitors: a review of electrode nanocomposites based on CNTs, graphene, metals, and polymers. *Symmetry*. 2023;15(6):1179. DOI:10.3390/sym15061179

7. Soni SK, Thomas B, Kar VR. A comprehensive review on CNTs and CNT-reinforced composites: syntheses, characteristics and applications. *Materials Today Communications*. 2020;25:101546. DOI:10.1016/j.mtcomm.2020.101546

8. Green MJ, Behabtu N, Pasquali M, Adams WW. Nanotubes as polymers. *Polymer*. 2009;50(21):4979-4997. DOI:10.1016/j.polymer.2009.07.044

9. Grady BP. *Carbon nanotube-polymer composites: manufacture, properties and applications*. New Jersey: Ballet; 2011. 352 p. DOI:10.1002/9781118084380

10. Yesil S, Bayram G. Poly(ethylene terephthalate)/carbon nanotube composites prepared with chemically treated carbon nanotubes. *Polymer Engineering & Science*. 2011;51(7):1286-1300. DOI:10.1002/pen.21938

11. Ribeiro B, Botelho EC, Costa ML, Bandeira CF. Carbon nanotube buckypaper reinforced polymer composites: a review. *Polímeros*. 2017;27(3):247-255. DOI:10.1590/0104-1428.03916

12. Koch W, Holthausen MC. *A chemist's guide to density functional theory*. Wiley; 2001. DOI:10.1002/3527600043

13. Rahman MdM, Mustakim S, Ullah MH, Islam MR, et al. Carbon nanotube and conducting polymer reinforced biomaterials for flexible supercapacitor electrodes toward sustainable energy storage. *Journal of Energy Storage*. 2026;162:122060. DOI:10.1016/j.est.2026.122060

14. Ali A, Rahimian Koloor SS, Alshehri AH, Arockiarajan A. Carbon nanotube characteristics and enhancement effects on the mechanical features of polymer-based materials and structures – a review. *Journal*

of Materials Research and Technology. 2023;24:6495-6521. DOI:10.1016/j.jmrt.2023.04.072

15. Ullah A, Hussain J, Waqar M, Humayun M, et al. Optimizing oxygen reduction efficiency with a robust nickel nitrogen-doped carbon nanotube catalyst for polymer electrolyte membrane fuel cells. *Results in Chemistry*. 2026;19:102918. DOI:10.1016/j.rechem.2025.102918

16. Elbakyan LS, Hayrapetyan DB, Mantashyan PA. DFT study of GaAs quantum dot and 5CB liquid crystal molecule interaction. *Journal of Molecular Graphics and Modelling*. 2025;136:108953. DOI:10.1016/j.jmgm.2025.108953

17. Chen Z, Nagase S, Hirsch A, Haddon RC, et al. Side-Wall opening of single-walled carbon nanotubes (SWCNTs) by chemical modification: a critical theoretical study. *Angewandte Chemie International Edition*. 2004;43(12):1552-1554. DOI:10.1002/anie.200353087

18. Dinadayalane TC, Leszczynski J. Stone-Wales defects with two different orientations in (5, 5) single-walled carbon nanotubes: a theoretical study. *Chemical Physics Letters*. 2007;434(1-3):86-91. DOI:10.1016/j.cplett.2006.11.099

19. Budyka MF, Zyubina TS, Ryabenko AG, Lin SH, et al. Bond lengths and diameters of armchair single wall carbon nanotubes. *Chemical Physics Letters*. 2005;407(4-6):266-271. DOI:10.1016/j.cplett.2005.03.088

20. Zaporotskova IV, Vilkeeva DE, Elbakyan LS. Sensor activity of titanium dioxide nanotubes in relation to acetone molecules. *Journal of Physics: Conference Series*. 2021;1967(1):012048. DOI:10.1088/1742-6596/1967/1/012048

21. Kumar S, Sharma A, Cherwoo L, Thombare N, et al. DFT study on the polymerization mechanism of aleuritic acid and jalaric acid in shellac molecule. *Kuwait Journal of Science*. 2024;51(1):100138. DOI:10.1016/j.kjs.2023.10.005

22. Akman F, Çankaya N. A study of experimental and theoretical analysis of N-cyclohexylmethacrylamide monomer based on DFT and HF computations. *Pigment & Resin Technology*. 2016;45(5):301-307. DOI:10.1108/PRT-04-2015-0039

23. Gao Y, Zhang J, Liang J, Yuan D, et al. Research progress of poly(methyl methacrylate) microspheres: preparation, functionalization and application. *European Polymer Journal*. 2022;175:111379. DOI:10.1016/j.eurpolymj.2022.111379

24. Jain P, Thakor S, Joshi A, Chauhan KV, et al. Machine learning-driven analysis of dielectric response in polymethyl methacrylate nanocomposites reinforced with multi-walled carbon nanotubes. *Journal of Materials Science: Materials in Electronics*. 2024;35(20):1419. DOI:10.1007/s10854-024-13188-x

25. Jindal P, Sain M, Kumar N. Mechanical characterization of PMMA/MWCNT composites under static and dynamic loading conditions. *Materials Today: Proceedings*. 2015;2(4-5):1364-1372. DOI:10.1016/j.matpr.2015.07.055

26. Mohamadian N, Ramhormozi MZ, Wood DA, Ashena R. Reinforcement of oil and gas wellbore cements with a methyl methacrylate/carbon-nanotube polymer nanocomposite additive. *Cement and Concrete Composites.* 2020;114:103763. DOI:10.1016/j.cemconcomp.2020.103763

27. David OB, Banks-Sills L, Aboudi J, Fourman V, et al. Evaluation of the mechanical properties of PMMA reinforced with carbon nanotubes – experiments and modeling. *Experimental Mechanics*. 2014;54(2):175-186. DOI:10.1007/s11340-013-9792-8

28. Navidfar A, Azdast T, Karimzad Ghavidel A. Influence of processing condition and carbon nanotube on mechanical properties of injection molded multi-walled carbon nanotube/poly(methyl methacrylate) nanocomposites. *Journal of Applied Polymer Science*. 2016;133(31):43738. DOI:10.1002/app.43738

29. Yuan H, Xiong Y, Shen Q, Luo G, et al. Synthesis and electromagnetic absorbing performances of CNTs/PMMA laminated nanocomposite foams in X-band. *Composites Part A: Applied Science and Manufacturing*. 2018;107:334-341. DOI:10.1016/j.compositesa.2018.01.024

30. Zhou D, Yu Z, Yuan H, Luo G, et al. Achieving wideband electromagnetic wave absorbing performance for PMMA-based composites foam by designing the alternating directional (Ad) microporous structure. *Materials Today Advances.* 2023;19:100395. DOI:10.1016/j.mtadv.2023.100395

31. Liu H, Yang Y, Tian N, You C, et al. Foam-structured carbon materials and composites for electromagnetic interference shielding: design principles and structural evolution. *Carbon.* 2024;217:118608. DOI:10.1016/j.carbon.2023.118608

32. Zhou D, Yuan H, Yu Z, Guo W, et al. Broadband electromagnetic absorbing performance by constructing alternate gradient structure (AGS) for PMMA-based foams. *Composites Part A: Applied Science and Manufacturing*. 2021;149:106578. DOI:10.1016/j.compositesa.2021.106557

33. Tan WK, Matsubara Y, Yokoi A, Kawamura G, et al. Transparent conductive polymer composites obtained via electrostatically assembled carbon nanotubes-poly (methyl methacrylate) composite particles. *Advanced Powder Technology*. 2022;33(4):103528. DOI:10.1016/j.apt.2022.103528

34. Muhammad Imran S, Go GM, Hussain M, Al-Harthi MA. Multiwalled carbon nanotube-coated poly-methyl methacrylate dispersed thermoplastic polyurethane composites for pressure-sensitive applications. *Macromol.* 2022;2(2):211-224. DOI:10.3390/macromol2020014

35. Blokhin A, Stolyarov R, Burmistrov I, Gorshkov N, et al. Increasing electrical conductivity of PMMA-MWCNT composites by gas phase iodination. *Composites Science and Technology*. 2021;214:108972. DOI:10.1016/j.compscitech.2021.108972

36. Kuromatsu S, Watanabe T, Nonoguchi Y, Suga R, et al. Single-wall carbon nanotube-based flexible monopole antenna fabricated using poly (methyl methacrylate)-supported transfer technique. In: *2022 Asia-*

Pacific Microwave Conference (APMC). Yokohama, Japan: IEEE; 2022. p. 866-868. DOI:10.23919/APMC55665.2022.9999853

37. Ziani D, Belkheir M, Rouissat M, Mokaddem A. Design optimization for microstrip antennas based on polymethyl methacrylate (PMMA) substrate and carbon nanotube (CNT) conductive material in sub-6 Ghz band. *Beni-Suef University Journal of Basic and Applied Sciences*. 2024;13(1):26. DOI:10.1186/s43088-024-00486-w

38. Patrignani M, Juan J, Nagel O, Reimers W, et al. The adsorption of CO and NO on (8,0) SWCNT decorated with transition metals: a DFT study as a possible gas sensor. *Powder Technology*. 2024;438:119691. DOI:10.1016/j.powtec.2024.119691

39. Islam MdA, Hossain N, Ahsan Z, Rana M, et al. DFT insights into the mechanical properties of NMs. *Results in Surfaces and Interfaces*. 2025;18:100417. DOI:10.1016/j.rsurfi.2025.100417

40. Krunić D, Armaković S, Bilić A, Armaković SJ, et al. Understanding the interactions between PMMA polymer and common industrial gasses: a computational xTB, DFT, SAPT and MD study. *Molecular Physics*. 2025;123(17):e2456108. DOI: 10.1080/00268976.2025.2456108

41. Krunić D, Armaković S, Yang Y, Bilić A, et al. Multiscale atomistic insights into interactions between PMMA and environmentally relevant β-blockers in an aqueous environment. *Molecular Simulation*. 2026; 52(8):646-661. DOI:10.1080/08927022.2026.2659203

42. Raj A, Alvi SMAA, Islam K, Motalab M, et al. An atomistic study of the tensile deformation of carbon nanotube-polymethylmethacrylate composites. *Polymers*. 2023;15(13):2956. DOI:10.3390/polym15132956

43. Zaporotskova IV, Elbakyan LS. Obtaining new dental materials reinforced with carbon nanotubes. In: *Advanced Technologies, Equipment, and Analytical Systems for Materials Science and Nanomaterials: Proceedings of the XI International Conference, Kursk, May 13-15, 2014.* Kursk: Southwestern State University; 2014. p. 325–326.

44. Zaporotskova IV, Elbakyan LS. New dental materials reinforced by carbon nanotubes: the technology of obtaining and the study of properties. *Vestnik Volgogradskogo gosudarstvennogo universiteta. Innovatsionnaya deyatel'nost'*. 2014;6(15):87-94. DOI:10.15688/jvolsu10.2014.6.8 (In Russ.)

45. Zaporotskova IV, Elbakyan LS. The possibility of creating polymer nanocomposites based on methacrylic acid by reinforcing them with carbon nanotubes. *Yevraziyskiy Soyuz Uchenykh. Seriya: Tekhnicheskiye i fiziko-matematicheskiye nauki.* 2014:39-42. (In Russ.)

46. Elbakyan L, Zaporotskova I. Experimental and DFT study of the conductive properties of PMMA composite material by doping with carbon nanotubes. *Nano-Structures & Nano-Objects*. 2025;44:101568. DOI:10.1016/j.nanoso.2025.101568

47. Zaporotskova IV, Elbakyan LS. The mechanism of interaction of esters of methacrylic acid with carbon nanotubes to create a new polymer composite material. *Journal of Nano- and Electronic Physics*. 2016; 8(3):03047-1-03047-3. DOI:10.21272/jnep.8(3).03047

48. Elbakyan LS, Zaporotskova IV, Vilkeeva DE. The mechanism of getting new composite polymer materials with improved hardness properties. *Key Engineering Materials.* 2021;887:85-90. DOI:10.4028/www.scientific.net/KEM.887.85

49. Elbakyan LS, Zaporotskova IV. Investigation of the effect of boron substitution impurities in carbon nanotubes on the interaction of polymethylmethacrylate with borocarbon nanotubes. *Fiziko-khimicheskiye aspekty izucheniya klasterov, nanostruktur i nanomaterialov.* 2025;17:906-915. DOI:10.26456/pcascnn/2025.17.906 (In Russ).

50. Hossain MdT, Shahid MdA, Mahmud N, Habib A, et al. Research and application of polypropylene: a review. *Discover Nano*. 2024;19(1):2. DOI:10.1186/s11671-023-03952-z

51. Patil J, Patil H, Sankpal R, Rathod D, et al. Studies on mechanical and thermal performance of carbon nanotubes/polypropylene nanocomposites. *Materials Today: Proceedings*. 2021;46:7182-7186. DOI:10.1016/j.matpr.2020.11.452

52. Sahli M, Barrière T, Roazard X, Assoul M. Investigating mechanical, thermal and rheological properties of polypropylene/carbon nanotubes composites. *Microsystem Technologies*. 2020;26(9):3023-3027. DOI:10.1007/s00542-020-04833-6

53. Bisht PS, Arora G, Pathak H. Strain-rate sensitivity analysis of microwave processed polypropylene-carbon nanotube composites. *Journal of Engineering Research*. 2026;14(1):237-245. DOI:10.1016/j.jer.2024.04.022

54. Thangavel S, Rajkumar D S, Jagadesh P. The impact of multi walled carbon nanotubes on the mechanical properties of polypropylene fibre reinforced concrete. *Case Studies in Construction Materials*. 2026;24:e05949. DOI:10.1016/j.cscm.2026.e05949

55. Hassanzadeh-Aghdam MK, Mahmoodi MJ, Ansari R. Creep performance of CNT polymer nanocomposites -An emphasis on viscoelastic interphase and CNT agglomeration. *Composites Part B: Engineering*. 2019;168:274-281. DOI:10.1016/j.compositesb.2018.12.093

56. Wu C, Wu R, Tam L ho. The creep behavior of semicrystalline carbon nanotube/polypropylene nanocomposite: a coarse-grained molecular study. *Polymer Degradation and Stability*. 2022;196:109834. DOI:10.1016/j.polymdegradstab.2022.109834

57. Sabet M. Enhancing the thermal and crystallization properties of polypropylene through carbon nanotube integration: a comprehensive investigation. *Iranian Polymer Journal*. 2024;33(6):727-741. DOI:10.1007/s13726-024-01278-w

58. Li Y, Lin J, Gao Y, Su Y. Regulation mechanism of hard-elastic behavior of polypropylene fibers by multiwalled carbon nanotubes. *Journal of Applied Polymer Science.* 2025;142(47):e57825. DOI:10.1002/app.57825

59. Ameli A, Nofar M, Park CB, Pötschke P, et al. Polypropylene/carbon nanotube nano/microcellular

structures with high dielectric permittivity, low dielectric loss, and low percolation threshold. *Carbon*. 2014;71:206-217. DOI:10.1016/j.carbon.2014.01.031

60. Gulrez SKH, Ali Mohsin ME, Shaikh H, Anis A, et al. A review on electrically conductive polypropylene and polyethylene. *Polymer Composites*. 2014;35(5):900-914. DOI:10.1002/pc.22734

61. Zhao K, Li S, Huang M, Shi X, et al. Remarkably anisotropic conductive MWCNTs/polypropylene nanocomposites with alternating microlayers. *Chemical Engineering Journal*. 2019;358:924-935. DOI:10.1016/j.cej.2018.10.078

62. Li C, Jiao Z, Xiong L, Yang W. Electrical conductivity of carbon nanotube/polypropylene composites prepared through microlayer extrusion technology. *Journal of Polymer Engineering*. 2017;37(8):795-804. DOI: 10.1515/polyeng-2016-0040

63. Bauhofer W, Kovacs JZ. A review and analysis of electrical percolation in carbon nanotube polymer composites. *Composites Science and Technology*. 2009; 69(10):14861498. DOI:10.1016/j.compscitech.2008.06.018

64. Tiwari SKr, Mishra J, Hatui G, Nayak GC. Conductive polymer composites based on carbon nanomaterials. In: Kumar V, Kalia S, Swart HC. (eds). *Conducting Polymer Hybrids*. Cham: Springer International Publishing; 2017. p. 117-142. DOI: 10.1007/978-3-319-46458-9_4

65. Stanciu NV, Stan F, Sandu IL, Fetecau C, et al. Thermal, rheological, mechanical, and electrical properties of polypropylene/multi-walled carbon nanotube nanocomposites. *Polymers*. 2021;13(2):187. DOI:10.3390/polym13020187

66. Kang D, Hwang S, Jung B, Shim J. Characterizations of polypropylene/single-walled carbon nanotube nanocomposites prepared by the novel melt processing technique with a controlled residence time. *Processes.* 2021;9(8):1395. DOI:10.3390/pr9081395

67. Wang J, Kazemi Y, Wang S, Hamidinejad M, et al. Enhancing the electrical conductivity of PP/CNT nanocomposites through crystal-induced volume exclusion effect with a slow cooling rate. *Composites Part B: Engineering*. 2020;183:107663. DOI:10.1016/j.compositesb.2019.107663

68. Zaccone M, Armentano I, Cesano F, Scarano D, et al. Effect of injection molding conditions on crystalline structure and electrical resistivity of PP/MWCNT nanocomposites. *Polymers*. 2020;12(8):1685. DOI: 10.3390/polym12081685

69. Alimoradi Y, Nourisefat M, Farzaneh A, Nazokdast H. Concurrent effect of shear flow and CNT presence on crystallization behavior and electrical properties of polypropylene based nanocomposites: a comprehensive structure-property investigation. *Journal of Composite Materials*. 2024;58(13):1589-1604. DOI: 10.1177/00219983241245998

70. Guo Y, Zhang D, Zhang X, Wu Y. Thermal properties and mechanical behavior of functionalized carbon nanotube-filled polypropylene composites using molecular dynamics simulation. *Materials Today Communications*. 2023;37:107510. DOI:10.1016/j.mtcomm.2023.107510

71. Wu C, Wu R, Tam L ho. Coarse-grained molecular simulation of the effects of carbon nanotube dispersion on the mechanics of semicrystalline polymer nanocomposites. *Nanotechnology.* 2021;32(32):325705. DOI:10.1088/1361-6528/abf458

72. Zaporotskova IV, Elbakyan LS, Vilkeeva DE. Strengthening of polymer ropes based on polypropylene with carbon nanotubes. *Journal of Physics: Conference Series*. 2021;1967(1):012047. DOI:10.1088/1742-6596/1967/1/012047

73. Elbakyan LS, Zaporotskova IV. Polypropylene modified with carbon nanomaterials: structure, properties and application (a review). *Polymers*. 2025;17(4):517. DOI:10.3390/polym17040517

74. Elbakyan LS, Zaporotskova IV. Mechanism for creating a composite based on polypropylene modified with carbon nanotubes of various layer degree. *Izvestiya vysshikh uchebnykh zavedeniy. Materialy elektronnoy tekhniki*. 2025;28(1):15-24. DOI:10.17073/1609-3577j.met202501.646 (In Russ.)

Information about the authors / Информация об авторах

Lusine S. Elbakyan, Cand. Sc. (Phys. and Math.), Associate Professor, Volgograd State University, Volgograd, Russian Federation; ORCID 0009-0006-1014-240X; e-mail: lusniak-e@yandex.ru

Элбакян Лусине Самвеловна, кандидат физико-математических наук, доцент, Волгоградский государственный университет, Волгоград, Российская Федерация; ORCID 0009-0006-1014-240X; e-mail: lusniak-e@yandex.ru

Received 06 April 2026; Revised 11 May 2026; Accepted 18 May 2026