ABSTRACT

of the dissertation work submitted for the degree of Doctor of Philosophy (PhD) in the educational program 8D05301- “Physics”

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Modeling of the transport properties of electronic nanodevices based on fullerene-like materials

Relevance of the topic

Nanotechnology is developing rapidly, having a revolutionary impact on various scientific fields, including microelectronics and optoelectronics. The potential applications of nanoscale materials are being actively explored in these areas. The flexibility of semiconductor materials has been a catalyst for the explosive growth of the semiconductor industry in recent decades. Moore's Law states that the computing power or speed of a microprocessor doubles every one and a half to two years, due to the constant increase in the number of transistors per unit area of a semiconductor chip. This trend has become the norm and goal of semiconductor technology and manufacturing development. However, the limit of computing power has not yet been reached. Advanced chip technologies aim to develop nanoelectronic devices that will overcome the limitations of miniaturization of traditional transistors and open the way to new generations of devices based on alternative principles. The materials and devices in nanoelectronics are so small that it is necessary to take into account interatomic contacts and the quantum mechanical properties of these materials. With the rapid development of miniaturization and scalable integration in the microelectronics industry, the development and production of miniature materials with desired mechanical, electrical, thermal and optical properties remains a key challenge.

In an effort to create increasingly compact and high-performance electronic devices, fullerene-like nanomaterials, such as fullerenes, carbon nanotubes , graphenes and similar structures, are used as the elemental base of quantum technologies. After Novoselov in 2004 graphene with the thickness of a carbon atom was isolated, and vigorous research activity led to the isolation of many other layered materials. Today, a large family of two-dimensional materials have a wide range of physical properties, including insulators, semiconductors, metals, semimetals and superconductors, as well as the recently discovered two-dimensional ferromagnetic materials. More importantly, two-dimensional materials are extremely sensitive to external influences such as electric and magnetic fields, making them ideal candidates for applications in electronics, optoelectronics and spintronics.

Over the past few years, fullerene-like materials have occupied a special niche in modern science, focusing on their unique properties, which open up new possibilities for application in condensed matter physics and beyond. The unique structure of fullerenes is justified by the fact that its atomic configuration can contain atoms, molecules, and other substances within its framework. This discovery was a real breakthrough in science, as it represents a new molecular

form of existence of carbon. The unusual properties of fullerenes determine the interest in them from researchers both from the point of view of fundamental science and for potential applied applications.

Carbon nanotubes (CNTs) are a revolutionary material that has unique properties. The use of carbon nanotubes in nanoelectronics is associated with their ultra-small sizes, which allows them to be used for miniaturization of products; they are also good current conductors. The emissive properties of CNTs make it possible to use them to create new light sources and displays. High chemical resistance makes nanotubes more resistant to environmental influences, and their ability to attach chemical radicals makes it possible to modify the properties to create new materials. It is also necessary to take into account that one of the main advantages of nanotubes is the quantum ballistic mechanism of conduction, which ensures the movement of electrons at low temperatures without scattering. Properties such as high carrier mobility, saturation drift rate, and ultra-low internal gate capacitance make carbon nanotubes an ideal material for radio frequency devices. Overall, carbon nanotubes have enormous potential for the development of future electronics.

The effect of correlated tunneling was predicted by scientists D.V. Averin and K.K. Likharev; the discovery of this phenomenon made a revolutionary contribution to the world of electronics and became the key to further miniaturization of electronic components. This phenomenon was based on Coulomb blockade, in which the movement of electrons is ordered under the influence of an electric field. Thanks to this effect, it became possible to create single-electron devices that use single molecules as the “nucleus”. Single-electron devices have a number of unique properties, such as low power consumption, high operating speed and ultra-high packaging density. In the future, single-electronics may revolutionize electronics, making it possible to create fundamentally new devices that will be much smaller, faster and more energy efficient than existing ones. Correlated tunneling of single electrons is a universal phenomenon that can be detected in a wide variety of materials. The list of such materials is extensive, including metals, semi- and superconductors, as well as carbon and molecular structures. Advances in the development of methods for characterizing and manipulating individual atoms and molecules, and progress in achieving first-principles modeling the process of electron tunneling through molecules has opened a new path to the development of the architecture of new nanoelectronic devices.

Studies of electronic states and transport properties are of great importance, both for understanding the physics of such small devices and for applications. The highlighting of quantum effects at the nanometer scale has opened up many areas of fundamental research, including nanoelectronics and spin electronics. Previous advances have led to important discoveries such as giant magnetoresistance and tunnel magnetoresistance in multilayer thin films, leading to significant advances in magnetic sensing and data storage. When integrating a ferromagnetic element into a single - electron transistor (SET), conditions arise under which it is possible to interact between the Coulomb blockade and the spin states of the electrons. Such

interactions can lead to the magnetocoulomb effect, which exhibits the properties of magnetotransport.

SETs are considered as a promising alternative to complementary metal oxide semiconductor technology due to low power consumption and high performance of sensitive sensors, memories, multi-logic devices, as well as in nanometrology and quantum computing. The latter promise to revolutionize technologies for generating and transmitting information. Unfortunately, a reliable and reproducible approach to the fabrication of devices remains the main bottleneck of nanoelectronics and nanospintronics, and the electronic devices themselves remain at the stage of laboratory research. Indeed, contacting and patterning individual nanoparticles with the required nanoscale precision is a very difficult technological task. At the same time, in large-scale devices with potentially thousands of nanoparticles in contact, having varying sizes and, therefore, different electronic properties, single-electron characteristics are smeared. Therefore, it is necessary to develop new materials and device concepts to overcome these difficulties.

The aim of the research work is to study the pattern of electric current flow through 0D, 1D and 2D van der Waals fullerene-like nanodevices using the example of endofullerene, polyprismane and bilayer graphenes using electron density functional theory in combination with the nonequilibrium Green's function method.

To achieve the aim, the following main tasks were set:

1. Search and selection of nanostructures with unique functional properties for the creation of electronic nanodevices, optimization of their geometry, construction of an adequate mathematical and computer model for calculating the behavior of nanostructures under the influence of an electric field.
2. Development of a model of a single-electron device based on endofullerenes, consisting of fullerenes with different diameters and interconnected by van der Waals forces, study of the mechanism of electron transport in such nanodevices.
3. Study of electronic transport in one-dimensional nanostructures using the example of polyprismanes with different diameters, interconnected by van der Waals forces, development of recommendations for the use of such materials for the creation of promising nanoelectronic devices.
4. Analysis and physical interpretation of the results obtained during a model study of nanodevices based on fullerene-like materials, identification of patterns of electric current flow in nanodevices based on van der Waals fullerene-like materials.

The object of the research work is zero-dimensional fullerene structures forming a core-shell nanojunction, one-dimensional coaxially connected prismane nanotubes, as well as moiré bilayer graphene films.

The subject of the research is the electrical transport properties of nanodevices based on fullerene-like materials .

Research Methods: This dissertation used a combined theory-based approach electron density functional together with the method of nonequilibrium Green's functions, which allows one to calculate the transport properties of

nanostructures and their electron densities. The density functional theory method is the main method for calculating the electronic structure of a many-particle system, which is based on the fact that any property of a system of interacting particles can be determined through the electron density functional. To achieve the set tasks, quantum chemical software systems were used for modeling and studying nanostructures, such as Atomistix ToolKit with Virtual NanoLab, Gaussian. When optimizing the geometry of the nanostructures under study within the framework of density functional theory, the generalized gradient approximation (GGA), exchange-correlation functionals PBE, and others were used. Visualization and correction of nanostructures was performed in the VESTA and GaussVIEW programs and mathematical calculation packages were also used. When calculating the total energy, electron density, charge stability diagram of single-electron devices, program codes written in Python were used.

Scientific novelty:

1. For the first time, a combination of fullerenes with different diameters has been modeled, leading to the manifestation of unique electrical properties, which makes it possible to increase the performance of single-electron transistors based on van der Waals 0D nanostructures: an increase in the number of resonance peaks in the transmission spectrum, the disappearance of the gap between the highest occupied molecular orbital and the lowest free molecular orbital, the appearance of indistinct step structures of Coulomb area on the current-voltage characteristic due to the weakening of the Coulomb energy, and also a decrease in the area of the Coulomb rhombus is noted on the stability diagram.

2. For the first time, a diode effect was discovered in polyprismane nanotubes ($C_{[14,17]}$-$C_{[14,11]}$-$C_{[14,5]}$), coaxially connected to each other by the van der Waals force, due to the formation of a Schottky barrier between the metal ($C_{[14,17]}$, $C_{[14,11]}$) and semiconductor ($C_{[14,5]}$) prisms .

3. It has been established that when passive graphene is twisted at moiré angles of ~4° and ~12° in an unstressed (and stressed) state, a modulated gap of ~1.66 eV and ~3.78 eV (~2.27 eV and ~4.28 eV), respectively, allowing to eliminate the disadvantage of gapless monolayer graphene for promising use as an elemental base for new quantum technologies.

The practical significance. The dissertation work is a theoretical study aimed at solving problems related to the study of electrotransport properties of fullerene-like structures. A number of fundamental results have been obtained, which have a practical orientation. The scientific results obtained in the study of the peculiarities of one-electron transport in conducting islands consisting of a combination of fullerenes with different diameters and separated by tunnelling transitions can be useful in the development of one-electron transistors based on them. Based on the proposed fullerene-like nanostructures, the fast performance of single-electron devices can be improved. The valve property of polyprismatic nanotubes ($C_{[14,17]}$-$C_{[14,11]}$-$C_{[14,5]}$) coaxially connected by van der Waals force can be used to design Schottky nanodiodes. A patent for a useful model of Schottky nanodiode has been obtained. The effect of opening of the modulated slit when twisting passive graphene to moiré angles in the unstressed and stressed state gives

the possibility of developing a component base of micro- and nanoelectronics with reduced power consumption on their basis.

The main provisions submitted for defense:

1. The combination of fullerenes with different diameters forming a core-shell nanojunction leads to an increase in the number of resonance peaks in the transmission spectrum, the disappearance of the gap between the highest occupied molecular orbital and the lowest unoccupied molecular orbital, and a decrease in the area of the Coulomb rhombus is noted on the stability diagram.

2. In coaxially interconnected polyprismane nanotubes ($C_{[14,17]}$ -$C_{[14,11]}$ - $C_{[14,5]}$) by the van der Waals force, a diode effect appears due to the formation of a Schottky barrier between the metal ($C_{[14,17]}$, $C_{[14,11]}$) and semiconductor ($C_{[14,5]}$) prisms .

3. When passive graphene is twisted at moire angles of ~4° and ~12° in the unstressed (and stressed) state, a modulated gap opens, the value of which varies from 1.66 - 1.82 eV and 3.78 - 4.69 eV (2.27 - 2.67 eV and 4.28 - 4.93 eV), respectively. The current-voltage characteristics of unstrained and stressed graphene have areas with negative differential conductivity, which manifests itself in different voltage values depending on the parameters of the moire structure.

The reliability of the obtained results is ensured by careful justification of the constructed computer models of nanodevices, observance of the limits of applicability of the used models and approximations for optimisation of the geometry of nanostructures, selection of correctness of computational methods for description of atomic and electronic structure of multi-atomic nano-systems, application of licensed computer programs Atomistix ToolKit with Virtual NanoLab, Gaussian, etc., approved by the international scientific community, as well as approbation in the form of publications in the international scientific journals.

Personal contribution of the author. Is that the whole scope of the dissertation work, the choice of research method, and problem solving were carried out by the author independently. Problem setting and discussion of the results were carried out jointly with scientific supervisors.

The connection of the topic with the plans of scientific works. This dissertation work was carried out within the framework of two research projects funded by the Ministry of Education and Science of the Republic of Kazakhstan, “The study of quantum-transport characteristics of nanosystems with unique operational electrical and magnetic properties” IRN AP08052562 for 2020-2022, as well as “Atomistic modeling of destruction semiconductor structures by electromagnetic pulses" IRN AR14869773 for 2022-2024.

Approbation of the research work. The results of the study were presented and discussed at international conferences:

1. 9th International Scientific and Practical Conference “Актуальные проблемы радиофизики” (Tomsk, Russia, September 20-22, 2021);

2. 10th International conference on Nanomaterials and Advanced Energy Storage Systems (Nur-Sultan, Kazakhstan, 4-6 August 2022);

The foreign internship took place at the Institute of Physics of the Ministry of Science and Education of Azerbaijan from 01/04/2023 to 02/05/2023, Baku, Azerbaijan.

Publications. By the results of the research presented in the dissertation work, published 6 scientific works, from of them: 3 articles indexed in Science Citation Index Expanded Web Database of Science, and in peer-reviewed scientific publications that have a percentile ranking according to CiteScore in the Scopus database ; 2 articles were published based on the results of international scientific and practical conferences in peer-reviewed scientific publications, having a percentile ranking according to CiteScore in the Scopus database, and 1 patent for a utility model.

1) Sergeyev D., Duisenova A., Solovjov A., Ismayilova N. Electron transport in a stressed moir´e bigraphene structure // Results in Physics. – 2023. – Vol. 54. – P. 107140. https://doi.org/10.1016/j.rinp.2023.107140 (Web of Science – Q1, Scopus – 89%).

2) Sergeyev D., Duisenova A. Electron transport in core-shell type fullerene nanojunction // Advances in Nano Research. – 2022. – Vol.12, № 1. – P. 25-35. https://doi.org/10.12989/anr.2022.12.1.025 (Web of Science – Q2, Scopus – 86%).

3) Sergeyev D.M. and Duisenova A.G. Electron Transport in Model Quasi-Two-Dimensional van der Waals Nanodevices // Technical Physics Letters. – 2021. – Vol. 47, № 4. – P. 417-420. [Сергеев Д. М., Дуйсенова А. Г. Электронный транспорт в модельных квази-двумерных ван-дер-ваальсовых наноустройствах // Письма в Журнал технической физики. – 2021. – Т. 47, №. 8. – С. 7-10. https://doi.org/10.21883/PJTF.2021.08.50844.18583]https://doi.org/10.1134/S1063785021040295 (Web of Science – Q4, Scopus – 36%)

4) Патент на полезную модель № 7120 РК. Нанодиод / Сергеев Д.М., Дуйсенова А.Г.; заявитель и патентообладатель НАО Актюбинский Региональный университет имени К. Жубанова. – № заявки 2022/0298.2; Дата заявки 07.04.2022; Опубликовано 20.05.2022, Бюл. № 20. – 7 с. URL: https://qazpatent.kz/en/content/poleznaya-model-20052022 . Дата обращения: 01.01.2024

5) Duisenova A., Sergeyev D. Model of single-electron transistor based on prismanes // Materials Today: Proceedings. – 2023. – Vol.81. – P.1192-1197. https://doi.org/10.1016/j.matpr.2022.11.175 (Scopus – 42%).

6) Duisenova A. G., Sergeyev D. M. Model of a single-electron transistor based on endohedral fullerene $(Sc_3N)@C_{80}$ // Journal of Physics: Conference Series. – IOP Publishing, 2021. – Vol. 2140, № 1. – P. 012006. https://doi.org/10.1088/1742-6596/2140/1/012006 (Scopus – 22%).

The structure and scope of the dissertation. This dissertation consists of an introduction, five sections, a conclusion and a list of sources used, corresponding to the stated purpose of the research, objectives and scope of the work performed. The work consists of 51 figures, 4 tables and a bibliography of 159 titles.

The main content of the dissertation.

The introduction presents the relevance of the dissertation work and its

basic provisions.

Conclusions on the first section:

The conducted literature review has shown that fullerene-like materials have unique electrophysical properties, which open up the possibility of creating new promising nanoelectronic devices based on them.

1. Fullerenes possess a framework structure that can encapsulate atoms and substances inside the carbon framework, depending on the properties of these encapsulated atoms, they can modify their electrical transport properties. Another feature of fullerenes is that they can accommodate small diameter fullerenes. Given that many fullerenes have metallic conductivity; it is possible to control the electrical capacity of a fullerene structure by selecting an encapsulated fullerene of the desired diameter. The special properties of fullerene include stability, the sublimation temperature of carbon atoms reaches 850 C°, they are wear resistant, the coefficient of friction is much lower than that of graphite, and they are thermally stable, withstanding heating to temperatures above 1000 C°, and the bulk modulus of elasticity reaches 668 GPa.
2. Polyprismans have a small cross section, in the form of a regular polygon, which favours the formation of a strong covalent bond. The increase in the effective diameter of polyprismane nanotubes leads to a change in their properties from metallic to semiconductor. They are wear-resistant, due to their rigid and strong structure, have high thermal stability, withstanding temperature values from 700 C °, elasticity, the value of Young's modulus of polyprismans is 100-200 GPa, hardness, reaching values of 10-15 GPa, which is comparable to the hardness of diamond.
3. Moiré graphenes, which are graphene films superimposed on each other at a certain small angle, bound together by the van der Waals force. The twisting angle of graphene in moiré graphene, can affect its electronic structure, in consequence of which they can have both metallic and semiconductor properties. At low temperatures, moiré graphenes can exhibit superconductor properties. These materials are relevant and interesting in the development of single-electron transistors and nanoelectronics devices.

Conclusions on the second section:

This section presents the theoretical foundations and methodological approaches underlying the computational modelling of the atomic structure of van der Waals fullerene-like materials and the prediction of their electrotransport properties using electron density functional theory in combination with the non-equilibrium Green's function method, considering the exchange-correlation functional and the generalised-gradient GGA-PBE approximation, as well as self-consistent field, energy balance, and molecular dynamics methods.

The choice of the DFT method provides a highly accurate calculation of the energy of a multielectronic system from first principles, requiring relatively small computational resources, while the use of the NRFG method is also based on first-principles methods, but has no free parameters, which excludes the possibility of ‘tuning’ the modelling results using empirical constants, and allows us to take into account the influence of fluctuations in the electron charge density during interactions between atoms.

The electrotransport properties of fullerene nanodevices have been modelled taking into account the theory of one-electron tunnelling, since tunnelling transitions are formed between the electrodes of the nanodevice and the fullerene molecule placed between them. The semi-empirical Kaasbjerg-Stokbro model was also applied, which allows the calculation of the electrical characteristics of one-electron transistors, taking into account the strong and weak coupling modes between the electrodes and the island.

Along with the outlined features of DFTs, computational methods for determining the electron density, total energy, and stability diagrams of nanostructures are also given.

Conclusions on the third section:

In this section, we present the results of the electrical transport properties of the model nanojunctions «Au–C_{180}–Au», «Au–C_{80}@C_{180}–Au» and «Au–(C_{20}@C_{80})@C_{180}–Au» in the framework of DFT combined with NRFG method and obtain the following results:

1. An increase in the number of resonance peaks of the transmission spectrum was found when small radius C_{20}, C_{80} fullerenes were introduced into the cavity of C_{180} fullerene, which shows an improvement in the electrical conductivity of such nano-objects. In the interval from -0.45 eV to 0.45 eV, a HOMO-LUMO gap is formed on the transmission spectrum of the Au-C180-Au nanojunction and its width is 0.9 eV. However, when small-sized fullerenes are introduced into C_{180}, this gap disappears and a series of peak resonance structures appear on the transmission spectrum of the C_{80}@C_{180}- , (C_{20}@C_{80})@C_{180}- nanojunctions.

2. It is shown that distinct step structures of Coulomb origin appear on the voltammetric characteristic of the C_{180}-nanojunction. On the CVC of C_{80}@C_{180}- , (C_{20}@C_{80})@C_{180}- nanojunctions, these step structures are ‘smeared’ due to the weakening of the Coulomb energy associated with the increase in the intrinsic electric capacities of the molecules.

3. It is found that on the dI/dV differential conductivity spectrum of the C_{180}-nanojunction there appear 8 peak structures of Coulomb origin with a period of 0.73 V, and on the spectrum of the C_{80}@C_{180}- , (C_{20}@C_{80})@C_{180}- nanojunctions 7 peak structures with periods of 0.74 V and 0.61 V, respectively.

4. It is shown that a large voltage is required at the source-to-source electrodes to bring the C_{180}-SETs out of the Coulomb blockade regime compared to transistors based on C_{80}@C_{180}- , (C_{20}@C_{80})@C_{180}- nanojunctions. The reduction of the Coulomb diamond area on the charge stability diagram of C_{80}@C_{180}- , (C_{20}@C_{80})@C_{180}-SETs allows to increase the fast performance of integrated circuits based on them.

The modelling results and the obtained data can be useful in the design of fast single-electron nanodevices. The obtained results open new opportunities for the purposeful design of fullerene nanotransitions of the ‘core-shell’ type with specified electrotransport characteristics, which have practical application in the development of high-tech nanoelectronics devices.

Conclusions on the fourth section:

In this section, a study on the electrotransport characteristics of telescopic prismatic C[14,17] - C[14,11] - C[14,5] nanotubes within the framework of TFG+NRFG was carried out and the following results were obtained:

1. It has been shown that the connection of telescoping polyprismanes in the form of nanotubes with different cross sections leads to a significant change in their electrical properties. In the transmission spectrum of telescoping polyprismanes $C_{[14,17]} - C_{[14,11]} - C_{[14,5]}$ in the range from -0.5 eV to 2.2 eV, an energy gap is formed between the HOMO-LUMO, the width of which is 2.7 eV.

2. The formation of stepped sections in the form of "Coulomb stairs" on the current-voltage characteristics of polyprismanes $C_{[14,17]} - C_{[14,11]}$, which are observed in single-electron devices due to the Coulomb blockade effect, was noted.

3. It is found that the coaxial coupling of polyprismans with different types of electrical conductivity, such as $C_{[14,11]} - C_{[14,5]}$ leads to the formation of Schottky barrier and manifestation of diode effect. From the density of state of polyprismans, it was clear that polyprismans $C_{[14,17]}$ and $C_{[14,11]}$ have metallic properties, whereas polyprisman $C_{[14,5]}$ exhibits the characteristics of a semiconductor with a forbidden zone of 0.4 eV.

The knowledge of the peculiarities of the electrical properties of telescoping prismatic nanotubes given in this section is important for the development of high-performance nanoelectronics devices, and can be useful in the calculations of Schottky nanodiodes.

Conclusions on the fifth section:

This section presents the results of modelling the electrical transport properties of unstressed, stressed and highly stressed moiré bigraphane nanodevices consisting of two layers of graphene, where one layer of graphene is electrically contacted with electrodes and the other remains electrically neutral, and the following scientific results are obtained: it has been revealed that the features of the band structure of the *K* point at the Fermi level in a stressed bilayer graphene system are preserved, but in a highly stressed state they change radically, apparently, this is due to a change in the bond between carbon atoms from vdW to covalent.

1. It has been established that when passive graphene is twisted at certain angles (~ 4° and ~ 12°) in an unstressed (and stressed) state, an energy gap opens, the value of which varies from 1.66 - 1.82 eV and 3.78 - 4.69 eV (2.27 - 2.67 eV and 4.28 - 4.93 eV), respectively.

2. It is shown that the transmission spectrum of bilayer graphene has a peak structure and is an order of magnitude lower than that of single-layer graphene.It is also found that when the graphene distance is reduced by 2.85 Å, the peak structures start to blur and their quasi-periodic behaviour is partially broken.It is also found that in the unstressed state at twisting passive graphene at $\theta = 4°$ in the range of bias voltage from 0 V to 1.1 V there is a gradual increase in the current up to ~10 μA, then a sharp increase in the current up to ~185 μA with the appearance of weakly expressed area of NDC, and at $\theta = 12°$ in the range of bias voltage from 1.35 V to 3 V there is a linear increase in the current up to ~220 μA. In the interval 0.4÷1.3 V, the CVC takes an *N*-shaped form, forming a pronounced NDC plot (-1.8 μSm at -0.71 V and 0.8 V). The same changes are also evident in the dI/dV

spectrum of the nanostructure and it was found that in the stressed state at θ = 4° there is a slight deviation from the unstressed state, and at θ = 12° the dI/dV spectrum becomes asymmetric, the -15 μSm NDC occurs only at positive voltage of 0.8 V, and at negative voltage the NDC is suppressed.

3. It is shown that in nanodevices consisting of a combination of graphene, silicene and molybdenum disulfide linked by van der Waals bonding, the interaction of silicene and molybdenum disulfide forms a new nanosystem predominantly with metallic properties, revealed on its transmission spectrum and WAC, it is also found that in the hybrid nanostructure «G – MoS_2 – Sil» a Schottky barrier is formed and it has rectifying diode properties.

The obtained data can be applied for the development and miniaturisation of high-performance transistors, for the creation of highly sensitive sensors of magnetic field, pressure and other substances.

In conclusion, the main results are presented:

The thesis presents the results of a modelling study of the electrical transport properties of fullerene-like structures (fullerene structures forming a nucleus-shell nanotransition, one-dimensional coaxially connected prismatic nanotubes, moiré bilayer graphene films). Let us list the most important results of the work done: During the dissertation work, the following results were achieved:

1. The combinations of «Au–C_{180}–Au», «Au–C_{80}@C_{180}–Au» and «Au–(C_{20}@C_{80})@C_{180}–Au» fullerenes with different diameters have been modelled, leading to the manifestation of unique electrical properties that allow to increase the fast performance of one-electron transistors based on van der Waals 0D nanostructures. The following phenomena are observed in such nano-objects: an increase in the number of resonant peaks of the transmission spectrum of endofullerenes, disappearance of the gap between the highest occupied molecular orbital and the lowest free molecular orbital; and the appearance of indistinct step structures of Coulomb origin on the voltammetric characteristic due to the weakening of the Coulomb energy, and a decrease in the area of the Coulomb diamond on the charge stability diagram.

2. It is shown that the coupling of telescoping polyprismans in the form of nanotubes with different cross sections leads to a significant change in their electrical properties: in the transmission spectrum of telescoping polyprismans $C_{[14,17]}$-$C_{[14,11]}$-$C_{[14,5]}$ in the range from -0.5 eV to 2.2 eV, an energy gap is formed between the highest occupied molecular orbital and the lowest free molecular orbital, the width of which is 2.7 eV; on the voltammetric characteristic of polyprismans $C_{[14,17]}$ – $C_{[14,11]}$ there appear stepped areas in the form of 'Coulomb ladders' due to the effect of Coulomb blockade; from the analysis of the density of state it is revealed that polyprismans $C_{[14,17]}$ and $C_{[14,11]}$ possess metallic properties, and polyprisman $C_{[14,5]}$ possesses semiconductor properties with a noticeable forbidden zone of 0.4 eV. The diode effect in polyprismane nanotubes ($C_{[14,17]}$-$C_{[14,11]}$-$C_{[14,5]}$) coaxially interconnected by van der Waals force is found due to the formation of Schottky barrier between the metallic ($C_{[14,17]}$, $C_{[14,11]}$) and semiconducting ($C_{[14,5]}$) prisms.

3. It is found that twisting the passive graphene to moiré angles of ~4° and ~12° in the unstressed (and stressed) state opens a modulated gap of ~1.66 eV

and ~3.78 eV (~2.27 eV and ~4.28 eV), respectively, which eliminates the disadvantage of slotless monolayer graphene for promising application as an elemental base of new quantum technologies. The voltammetric characteristic of unstressed and stressed graphene have regions with negative differential conductivity, manifested in different voltage values depending on the moiré structure parameters. It is found that in the stressed state at $\theta = 4°$ there is a slight deviation from the unstressed state, and at $\theta = 12°$ the dI/dV spectrum becomes asymmetric, the negative differential conductivity of -15 μSm occurs only at a positive voltage of 0.8 V, and at negative voltage the negative differential conductivity is suppressed.

Assessment of the completeness of the solutions to the set tasks. The tasks set in the dissertation work have been fulfilled in full, all modelling studies have been carried out and the conformity of the obtained results has been proved. The obtained results were discussed at seminars in the scientific centre «Radiation physics of materials» at Aktobe Regional University named after K. Zhubanov, as well as in international conferences.

Recommendations on the specific use of research results. The obtained fundamental results have practical significance. Scientific results are obtained in the study of the features of one-electron transport, and can be useful in the development of one-electron transistors based on fullerene-like materials.

Evaluation of the scientific level of the performed work in comparison with the best achievements in this field. High scientific level of the thesis work is provided by approbation in the form of 5 publications in international scientific journals of WoS and Scopus databases with high indicators (Q1, Q2), a patent for a useful model, and participation in international scientific conferences. The results of the thesis research were approved at two international scientific-practical conferences.

In conclusion, I express my deep gratitude to my scientific advisors Candidate of Physical and Mathematical Sciences, Professor Sergeev Daulet, Doctor of Physical and Mathematical Sciences, Professor Solovyov Andrey, PhD Ismailova Narmin for their invaluable support, and help in solving problems throughout the study, which was the key to the successful completion of the dissertation work.