Project name, IRN	**AP08052562 –** The study of quantum-transport characteristics of nanosystems with unique operational electrical and magnetic properties
Completion date	01.05.2020-31.12.2022
Project supervisor	Sergeyev Daulet Maksatuly – PhD, professor
Report	This project is aimed at studying the quantum transport characteristics of nanosystems with unique operational electrical and magnetic properties, which are nanoscale objects in the form of a molecule placed between metal (or semiconductor) electrodes (in a nanogap). Such objects act as basic active elements of nanoelectronics: nanodiodes, nanotransistors and others. However, the energy characteristics of nanodevices strongly depend on the slightest change in the geometric dimensions and electronic structures of molecules. The project (from first principles) will select nanostructures with unique operational electrical and magnetic properties to create nanodevices, and also study their quantum transport characteristics. As a result, new data on the quantum transport of nanosystems will be obtained. A search will be made for new nanostructures with unique electrical and magnetic properties to create nanodevices, their geometries are optimized using a generalized gradient approximation with different exchange-correlation functionals, adequate mathematical and computer models are constructed to calculate the behavior of nanostructures under the influence of an electric field. Models of electronic nanodevices - nanodiodes, nanoswitches, nanosensors - based on both single and complex molecules will be developed, optimal parameters will be selected and their main electrical transport characteristics will be calculated. The mechanisms of electron transport in single-electron transistors will be comprehensively investigated and their basic electrophysical characteristics determined. The features of the effect of spin-dependent transport in quasi-two-dimensional carbon nanostructures with various geometric shapes will be investigated and models of the spin filter based on them will be developed. The features of the effect of multiple Andreev reflection in superconducting nanostructures will be investigated. Obtained fundamental laws can be useful for creating new promising electronic devices of nanoelectronics. Scientific results on the study of the quantum transport properties of low-dimensional systems can be useful for miniaturization of electronic components of electronics.
Relevance	In recent years there has been intensive progress in electronics, with the miniaturisation of electronic components at its heart. Modern semiconductor electronics based on silicon and gallium arsenide have already reached their physical limit due to the fundamental characteristics of these materials. Therefore, nowadays, the development of new materials with controllable electro-physical properties becomes more important for the development of new types of micro- and nanoelectronic devices. In this regard, new areas of nanoelectronics based on exotic materials with fundamentally new electrophysical properties compared with conventional semiconductor materials are being

	developed. These nanoelectronics fields include superconductor, organic, molecular and single-electronics, where nanoscale structures are the working objects. At present, the development of nanoelectronics elements has slowed down because of certain problems, such as heat dissipation from 'inorganic' structures in ultra-dense atomic size elements, reduced power consumption and increased speed, compatibility of neural network elements and nanoelectronics elements, coupling of new circuit elements to a silicon platform, and high probability of macro-contact short-circuiting and breakdown. To solve these problems, comprehensive basic and applied research into the specifics of electronic transport mechanisms in nanostructures is needed. Therefore, the search for nanostructures with unique functional properties and the development of highly efficient nanodevices based on them is an urgent task for condensed matter physics and physical electronics. This project is devoted to the investigation and solution of problems arising in the design of promising nanoelectronics elements and theoretical analysis of quantum transport characteristics of such nanodevices.
Purpose	The goal of this project is within the framework of the electron density functional theory (from first principles), the nonequilibrium Green's function method (DFT + NEGF) and other numerical simulation methods: selection of nanostructures with unique functional properties to create efficient nanodevices; creation on their basis of various models of nanodevices - nanodiodes, nanotransistors, nanoswitches and others; study of quantum-transport characteristics of nanodevices, the study of their electrical and magnetic properties.
Expected results	– A search will be made for new nanostructures with unique electrical and magnetic properties to create nanodevices, optimized their geometries using the generalized gradient approximation (GGA) with exchange-correlation functionals PBE, B3LYP and others, constructed adequate mathematical and computer models to calculate the behavior of nanostructures under the influence electric field. – Models of electronic nanodevices - nanodiodes, nanoswitches, nanosensors - based on both single and complex molecules will be developed, optimal parameters will be selected and their main electrical transport characteristics will be calculated. – Mechanisms of electron transport in single-electron transistors based on endofullerenes, prismans and other nanomaterials using various computer simulation methods will be comprehensively investigated and their basic electrophysical characteristics will be determined. – The features of the spin-dependent transport effect in quasi-two-dimensional carbon nanostructures with different geometric shapes will be investigated and spin filter model developed based on them. – The features of the multiple Andreev reflection effect in superconducting nanostructures consisting of a combination of a superconductor with nanomaterials of various types of

	conductance will be investigated, and recommendations on the use of such nanostructures to create promising electronic cryoelectronics devices will be developed.
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Publications in scientific publications	1. Sergeyev D. Single Electron Transistor Based on Endohedral Metallofullerenes Me@C60 (Me = Li, Na, K) // Journal of Nano- and Electronic Physics. – 2020. – Vol. 12, No 3. – 03017. https://doi.org/10.21272/jnep.12(3).03017 2. Sergeyev D., Ashikov N., Zhanturina N. Electric transport properties of a model nanojunction “Graphene – Fullerene C60 – Graphene” // International Journal of Nanoscience. – 2021. – Vol. 20, No 1. – 21500071. https://doi.org/10.1142/S0219581X21500071 3. D. Sergeyev, N. Zhanturina, L. Myasnikova, A.I. Popov, A. Duisenova, A. Istlyaup. Computer simulation of the electric transport properties of the FeSe monolayer // Latvian journal of physics and technical sciences. – 2020. – Vol. 57, No 6. – P. 3-11. https://doi.org/10.2478/lpts-2020-0029 4. D. Sergeyev. Nanoswitch based on ring-opening of 1,3-cyclohexadiene molecule // International Journal of Nanoelectronics and Materials. – 2021. – Vol. 14, No 1. – P.49-60. 5. Sergeyev D. One-dimensional Schottky nanodiode based on telescoping polyprismanes // Advances in Nano Research. – 2021. – Vol. 10, No 4. – P. 339-347. https://doi.org/10.12989/anr.2021.10.4.339 6. Sergeyev D., Duisenova A. Electron Transport in Model

	Quasi-Two-Dimensional van der Waals Nanodevices // Technical Physics Letters. – 2021. – Vol. 47, No 4. – P. 375–378. https://doi.org/10.1134/S1063785021040295 7. Petrenko E.V., Omelchenko L.V., Kolesnichenko Yu.A., Shytov N.V., Rogacki K., Sergeyev D.M., Solovjov A.L. Study of fluctuation conductivity in YBa2Cu3O7–δ films in strong magnetic fields // Low Temperature Physics/Fizika Nizkikh Temperatur. – 2021. – Vol. 47, No 12. – P. 1148–1156.
Participation in a conference on the topic of the research	9th International Scientific and Practical Conference "Actual Problems of Radiophysics", 20-22 October 2021, Tomsk, Russia.