Project name, IRN	**AP23488734** – Ab-initio investigation on electronic and quantum transport properties of one-dimensional and two-dimensional van-der-Waals nanoheterodevices based on transition metal dichalcogenides
Completion date	01.01.2024-31.12.2026
Project supervisor	Sergeyev Daulet, Candidate of Physical and Mathematical Sciences professor
Report	With the development of the scientific and technological base of electronics, there is a gradual miniaturization of its electronic components, which in turn leads to functional and structural complexity of electronic systems, but an increase in their reliability and speed, a decrease in energy consumption, etc. A significant increase in placement density and reduction in the size of electronic components will most likely be possible on the basis of fundamentally new ideas. At present, prototypes of nanoelectronic devices with unique electrophysical characteristics have already been created. Work is actively underway to develop new areas of nanoelectronics. Van der Waals heterostructures, which are a set of isolated atomic planes connected with the Van der Waals force and assembled according to a pre-selected sequence, have been proposed as one of the promising materials for electronic technology. In recent years, the electronic and optical properties of van der Waals nanoheterostructures based on transition metal dichalcogenides have been intensively studied due to their attractiveness for the development of new quantum technologies, as well as the discovery of new fundamental quantum phenomena. The aim of this project is to develop atomistic models of one-dimensional and two-dimensional van der Waals nanoheterodevices based on transition metal dichalcogenides (TMDs) in combination with other graphene-like materials with different types of conductivity and study their electronic and quantum transport properties from first principles, including and under the influence of various factors (deformation, external electric field, moire potential, zero-dimensional defects, etc.). The project is aimed at a model study of the quantum transport properties of new one-dimensional and two-dimensional van der Waals TMD nanoheterodevices, including when they are exposed to various factors. To optimize the geometry of TMD nanoheterodevices, as well as determine their quantum transport characteristics, density functional theory will be used in combination with the nonequilibrium Green's function method. The project will develop atomistic models of one-dimensional and two-dimensional van der Waals nanoheterodevices based on transition metal dichalcogenides in combination with other nanomaterials with different types of conductivity, study the fundamental phenomena that determine their quantum transport characteristics, and study the features of their electronic properties under the influence of various factors (deformation, electric field, moiré potential, zero-dimensional defects, etc.), and research will also be carried out to develop models of sensitive nanoelements of sensor devices and solar cells.

Purpose	*The aim of project* is to develop atomistic models of one-dimensional and two-dimensional van-der-Waals nanoheterodevices based on transition metal dichalcogenides in combination with other graphene-like materials with different types of conductivity and study their electronic and quantum transport properties from first principles, including and under the influence of various factors
Expected results	• 1) based on the results of research conducted within the framework of this project, it is planned to publish at least 3 (three) articles and (or) reviews in peer-reviewed scientific journals in the scientific direction of the project, indexed in the Science Citation Index Expanded and included in 1 (first), 2 (second) and (or) 3 (third) quartile by impact factor in the Web of Science database and (or) having a CiteScore percentile in the Scopus database of at least 60 (sixty) (proposed publications: Results in Physics (Web of Science – Q1, Scopus – 89%), Advances in Nano Research (Web of Science – Q2, Scopus – 94%), Physica E: Low-dimensional systems and nanostructures (Web of Science – Q2, Scopus – 78%), IEEE Sensors Journal (Web of Science – Q1, Scopus – 90%), Crystals (Web of Science – Q2, Scopus – 54%), Electronic Materials Letters (Web of Science – Q3, Scopus – 70%), etc.); at least 1 (one) article or review in a peer-reviewed foreign or domestic publication recommended by Committee for Quality Assurance in the Field of Science and Higher Education (supposed publications: Eurasian Journal of Physics and Functional materials, Bulletin of the Karaganda University – Physics, or foreign scientific publications indexed in the Russian Science Citation Index and Emerging Sources Citation Index from Clarivate Analytics or Scopus database). • 2) there are no plans to publish monographs, books and (or) chapters in books from foreign and (or) Kazakh publishing houses; • 3) it is planned to apply for a patent for a utility model in the Kazakhstan patent Office; • 4) there are no plans to develop scientific, technical, design documentation; • 5) dissemination of the results of the work among potential users, the scientific community and the general public will be carried out in the form of scientific publications in peer-reviewed foreign and domestic journals, as well as in the form of participation in international scientific conferences; • 6) other measurable results in accordance with the requirements of the competition documentation and the features of the project: • 1) scope of application of the expected results: nanoelectronics, microelectronics, renewable energy; target consumers: research laboratories, higher education institutions. • 2) the fundamental results obtained during the study can be useful for the further development of active electronic components of nano- and microelectronics; • 3) applicability and (or) possibility of commercialization of the obtained scientific results; the obtained atomistic models of nanoheterostructures can be used to improve the efficiency of solar cells and sensitive elements of nanosensors; • 4) the identification of new quantum transport properties of nanoheterostructures based on transition metal dichalcogenides can be used to improve the output characteristics of existing electrical devices, and can also be taken into account when developing new types of electronic components;

	• 5) the results obtained can be applied to the development of new types of electronic components, sensors, and solar cells.
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List of published works	