Quantum Mechanics for Nanostructures

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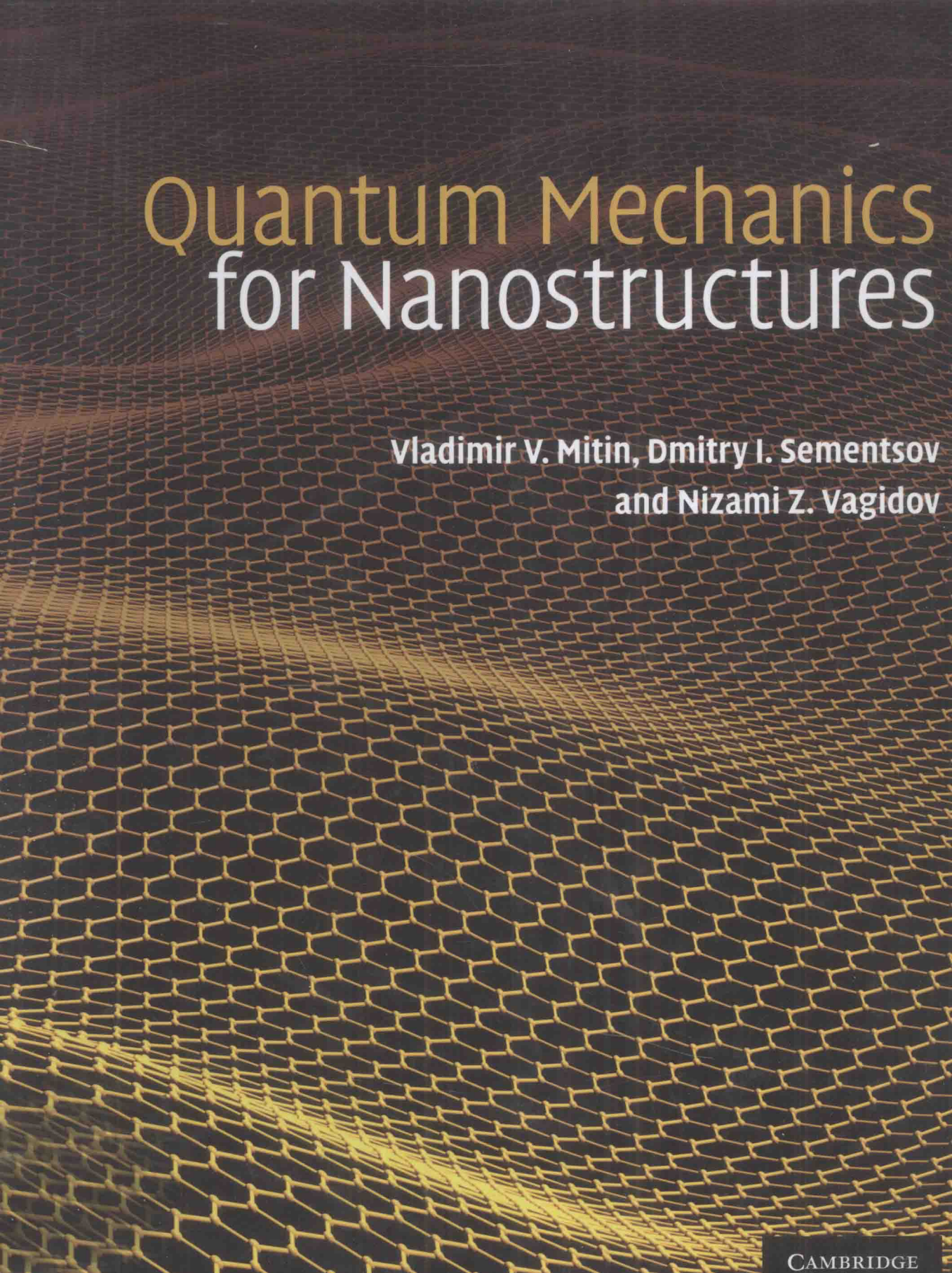
and Nizami Z. Vagidov



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Vladimir V. Mitin
University at Buffalo, The State University of New York

Dmitry I. Sementsov
Ulyanovsk State University

Nizami Z. Vagidov
University at Buffalo, The State University of New York

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Quantum Mechanics for Nanostructures

The properties of new nanoscale materials, their fabrication and applications, as well as the operational principles of nanodevices and systems, are solely determined by quantum-mechanical laws and principles. This textbook introduces engineers to quantum mechanics and the world of nanostructures, enabling them to apply the theories to numerous nanostructure problems.

The book covers the fundamentals of quantum mechanics, including uncertainty relations, the Schrödinger equation, perturbation theory, and tunneling. These are then applied to a quantum dot, the smallest artificial atom, and compared with the case of hydrogen, the smallest atom in nature. Nanoscale objects with higher dimensionality, such as quantum wires and quantum wells, are introduced, as well as nanoscale materials and nanodevices. Numerous examples throughout the text help students to understand the material.

Vladimir V. Mitin is SUNY Distinguished Professor at the Department of Electrical Engineering and Adjunct Professor of Physics at the University at Buffalo, The State University of New York. He is the author of eight textbooks and monographs and more than 490 professional publications and presentations.

Dmitry I. Sementsov is Professor of Physics at Ulyanovsk State University, Russia. He is the author of more than 420 papers in peer-reviewed journals.

Nizami Z. Vagidov is Research Assistant Professor of Electrical Engineering at the University at Buffalo, The State University of New York. He is the author of about 90 professional publications in the fields of solid-state electronics, nanoelectronics, and nanotechnology.

Preface

Nanoelectronics is a field of fundamental and applied science, which is rapidly progressing as a natural development of microelectronics towards nanoscale electronics. The modern technical possibilities of science have reached such a level that it is possible to manipulate single molecules, atoms, and even electrons. These objects are the building blocks of nanoelectronics, which deals with the processes taking place in regions of size comparable to atomic dimensions. However, the physical laws which govern electron behavior in nanoobjects significantly differ from the laws of classical physics which define the operation of a large number of complex electronic devices, such as, for example, cathode-ray tubes and accelerators of charged particles. The laws that govern electron behavior in nanoobjects, being of quantum-mechanical origin, very often seem to be very strange from a common-sense viewpoint. The quantum-mechanical description of electron (or other microparticle) behavior is based on the idea of the *wave–particle duality of matter*. The wave properties of the electron, which play a significant role in its motion in small regions, require a new approach in the description of the electron's dynamic state on the nanoscale. Quantum mechanics has developed a fundamentally new probabilistic method of description of particle motion taking into account its wave properties. This type of description is based on the notion of a wavefunction, which is not always compatible with the notion of a particle's trajectory. This makes electron behavior harder to understand.

The main objects of research in nanoelectronics are quantum-dimensional structures such as *quantum wells*, *quantum wires*, and *quantum dots*, where electron motion is limited in one, two, and three directions, respectively. The size of these quantum-mechanical objects is comparable to the *electron de Broglie wavelength*. In such structures electronic properties become different from those of bulk materials: new so-called low-dimensional effects become apparent. Quantum-mechanical laws govern various processes and define a significant modification of the energy spectrum, which is the main characteristic of an electronic system. The energy spectrum which characterizes the electron motion in the limited region becomes discrete. The structures with such an energy spectrum are the basis for the development of new types of nanoelectronic devices.

The physics of quantum-dimensional structures is currently developing rapidly and is beginning to form a separate field with quantum mechanics

as its basis. Only a small number of undergraduate engineering students take quantum-mechanics courses. However, there are only a few textbooks that are simple enough to understand for a wide range of engineering students, who would like to learn theoretical methods of analysis of the electronic properties of low-dimensional structures. While writing the current textbook we pursued two main goals: to present the main low-dimensional structures clearly from the physical point of view and to teach the reader the basics of quantum-mechanical analysis of the properties of such structures. Therefore, the experimental and theoretical material which will help the reader to understand the quantum-mechanical concepts applied to *nanostructures* is presented. Special attention is paid to the physical interpretation of quantum-mechanical notions. Theoretical material as well as the mathematical apparatus of quantum mechanics necessary for carrying out quantum-mechanical calculations independently is presented.

The book is written in such a way that it can be used by students who have studied classical physics to a sufficient extent as well as by students who have not had such an opportunity. The book consists of eight chapters and three appendices. The appendix material contains the main aspects of classical physics (particle dynamics, oscillations and waves in crystals, and electromagnetic fields and waves) which students can use while studying quantum mechanics.

In Chapter 1 we give a review of milestones in the development of *nanotechnology* and *nanoscience*. The main types of nanostructures are described and it is substantiated why it is necessary to use quantum physics for the description of their properties.

In Chapter 2 the main experimental facts which required the introduction of such unusual (for classical physics) notions as *wave–particle duality and uncertainty relationships*, among others, are described. The main notions and principles of the quantum-mechanical description are introduced. The Schrödinger equation – the main equation of non-relativistic quantum mechanics – is discussed in detail and its validity for the description of nanostructures is presented.

In Chapter 3 the solutions of the stationary Schrödinger equation are obtained for several important cases of one-dimensional motion. The main peculiarities of free electron motion as well as confined electron behavior are discussed. The main advantage of these solutions is in explanation and quantitative definition of the discrete energy levels of an electron when it moves in potential wells of various profiles.

In Chapter 4 the peculiarities of electron motion for structures wherein electron motion is confined in two and three dimensions are considered. It is shown that the discrete electron energy levels are characteristic for electron motion in potential wells of particular dimensionalities, in contrast to the continuous energy spectrum of a free electron. The structure's dimensionality and potential profile define the positioning of energy levels in the discrete energy spectrum.

The calculation of electron quantum states in various types of nanostructures generally encounters big mathematical difficulties. Therefore, approximate methods become very important for finding solutions of the Schrödinger equation. We consider in Chapter 5 several important and widely used approximate methods for calculation of electron wavefunctions, energy states, and transition probabilities between quantum states.

Chapter 6 is dedicated to finding wavefunctions, the geometry of electron clouds corresponding to them, and energy spectra of the simplest atoms and molecules using approximate methods.

When the size of the potential well is several times larger than the distance between atoms in a crystal, a fundamental reconstruction of the energy spectrum, which leads to a change in the physical properties of nanostructures, takes place. In Chapter 7 the main peculiarities of the electron energy spectrum in low-dimensional quantum structures (quantum wells, wires, and dots) as well as in periodic structures (superlattices) consisting of these low-dimensional nanostructures are considered.

In the last chapter – Chapter 8 – we consider the main methods of fabrication and characterization of nanostructures as well as their prospective applications in modern nanoelectronics.

Practically all chapters and appendices contain a large number of detailed examples and homework problems, which the authors hope will help students to acquire a deeper understanding of the material presented.

The authors have many professional colleagues and friends from different countries who must be acknowledged. Without their contributions and sacrifices this work would not have been completed. Special thanks go to the Division of Undergraduate Education of the National Science Foundation for the partial support of this work through its Course, Curriculum and Laboratory Improvement Program (Program Director Lance Z. Perez). The authors would like especially to thank Professor Athos Petrou for his editorial efforts in a critical reading of this book and for many valuable comments and suggestions. The authors also would like to thank undergraduate student Brian McSkimming for his thorough reading of the manuscript and helpful comments. We would like to thank undergraduate student Jonathan Bell for his help in preparation of figures.

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Notation

Symbols

A – amplitude
A_{wf} – work function
a – lattice constant
a – acceleration
$\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ – basis vectors
$\mathbf{B}$ – magnetic flux density
$\mathbf{C}$ – wrapping vector
C – capacitance
c – speed of light in vacuum
D – superlattice period
$\mathbf{D}$ – electric displacement
$\mathbf{d}$ – translation vector
E – energy of a particle
E_{c} – bottom of conduction band
E_{g} – bandgap
E_{i} – ionization energy
E_{v} – bottom of valence band
E_{F} – Fermi energy
$\mathbf{E}$ – electric field intensity
e – elementary charge
$\mathbf{e}_r$ – unit vector directed along radius vector $\mathbf{r}$
$\mathbf{e}_x$, $\mathbf{e}_y$, $\mathbf{e}_z$ – unit coordinate vectors
$\mathbf{F}_{\mathrm{gr}}$ – gravitational force
$\mathbf{F}_{\mathrm{L}}$ – Lorentz force
$\mathbf{F}_{\mathrm{m}}$ – magnetic force
$\mathbf{F}_{\mathrm{e}}$ – electric force
g – acceleration due to gravity; density of states
$\mathbf{H}$ – magnetic field intensity
H_n – Hermite polynomials
$\hat{\mathcal{H}}$ – Hamiltonian operator
h – Planck's constant
$\hbar$ – reduced Planck constant

I – current
I_{T} – tunneling current
$\mathbf{i}, \mathbf{j}, \mathbf{k}$ – unit coordinate vectors
K – kinetic energy; superlattice wavenumber
k – spring constant; wavenumber
$\mathbf{k}$ – wavevector
k_{B} – Boltzmann's constant
$k_{\mathrm{e}} = 1/(4\pi\epsilon_0)$ – coefficient in SI system
l – orbital quantum number
$\mathbf{L}$ – angular momentum
L_x, L_y, L_z – dimensions of a sample
m – orbital magnetic quantum number
m^* – effective mass of an electron
m_0 – mass of particle at rest
m_{e} – electron mass in vacuum
m_{s} – magnetic quantum number
N – number of states
N_{A} – Avogadro constant
n – principal quantum number; concentration
$\mathbf{P}$ – Poynting vector
$\mathcal{P}$ – pressure
P – probability
$\mathbf{p}$ – momentum
$\mathbf{q}$ – wavevector
Q – charge
q – charge of a particle
R – universal gas constant
r – magnitude of radius vector
r_1 – first Bohr radius
$\mathbf{r}$ – coordinate vector
R_∞ – Rydberg's constant
$\mathbf{R}_{\mathrm{c}}$ – radius vector of center of mass
$\mathbf{S}$ – spin
S – cross-section
t – time
T – time period; ambient temperature
$\mathcal{T}_{\mathrm{d}}$ – translation operator
U – potential energy; applied voltage
U_0 – height of potential barrier
U_{G} – gate voltage
u – displacement of atoms from their equilibrium positions
V – volume
v – velocity

v_{gr} – group velocity
v_{ph} – phase velocity
V_c – velocity of center of mass
W – work done by a force
$X(r)$ – radial function
x, y, z – spatial coordinates
Y_{ml} – spherical harmonics
α – angle; Madelung constant
β – force constant; $b/(2m)$
γ – gyromagnetic ratio
δ – logarithmic decrement of damping
$\delta(x)$ – Dirac's delta-function
ϵ – dielectric constant of the medium; relative deformation
ϵ_0 – permittivity of free space
ε – energy
ϕ – electrostatic field potential
φ – azimuthal angle; chiral angle; phase difference
λ – wavelength; parameter in characteristic equation
λ_{Br} – de Broglie wavelength
μ – magnetic permeability; magnetic moment
μ_l – orbital magnetic moment
μ_B – Bohr magneton
$\nabla^2 = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2} + \dfrac{\partial^2}{\partial z^2}$ – Laplace operator
ψ – stationary wavefunction
Ψ – time-dependent wavefunction
Ω – angular velocity of a particle
ω – frequency
ω_e – frequency of electron oscillations
ω_q – frequency of harmonic oscillator
ρ – three-dimensional density
$\boldsymbol{\tau}$ – torque
θ – polar angle

Contents

Chapter 1
The nanoworld and quantum physics

1.1 A review of milestones in nanoscience and nanotechnology

It is extremely difficult to write the history of nanotechnology for two reasons. First, because of the vagueness of the term "nanotechnology." For example, nanotechnology is very often not a technology in the strictest sense of the term. Second, people have always experimented with nanotechnology even without knowing about it. Ironically enough, we can say that the medieval alchemists were the founding fathers of nanoscience and nanotechnology. They were the first researchers who tried to obtain gold from other metals. The ancient Greek philosopher Democritus also can be considered as a father of modern nanotechnology, since he was the first to use the name "atom" to characterize the smallest particle of matter. The red and ruby-red opalescent glasses of ancient Egypt and Rome, and the stained glasses of medieval Europe, can be considered as the first materials obtained using nanotechnology. An exhibition at the British Museum includes the Lycurgus cup made by the ancient Romans. The glass walls of the cup contain nanoparticles of gold and silver, which change the color of the glass from dark red to light gold when the cup is exposed to light. In 1661 the Irish chemist Robert Boyle for the first time stated that everything in the world consists of "corpuscules" – the tiniest particles, which in different combinations form all the varied materials and objects that exist.

In modern history the first practical breakthrough in nanotechnology was made by the American inventor George Eastman, who in 1884 fabricated the first roll film for a camera. This film contained a photosensitive layer of silver bromide nanoparticles. In 1931 the German physicists Max Knoll and Ernst Ruska developed an electron microscope, which for the first time allowed one to study nanoobjects.

The development of modern optical, microelectronic, material science, chemical, biological, and other technologies, which took into account quantum-dimensional effects, and, subsequently, the development of the main concepts and methods for the formation and control of nanoparticles has accelerated at an

explosive rate. This development was based on the achievements and discoveries made by researchers in diverse fields of science.

The notion of "nanotechnology" was introduced for the first time by Richard Feynman in 1959 in his famous Caltech lecture "There's plenty of room at the bottom: an invitation to enter a new field of physics." Richard Feynman imagined the world of the nanoscale where the fundamental laws of quantum physics define the behavior of a single atom and control the formation of different structures from individual atoms. This vision of the great scientist ushered in the modern era of nanotechnology. The main achievements of this era are the following.

In 1952, L. V. Radushkevich and V. M. Lukyanovich published the first clear images of 50-nm-diameter carbon nanotubes. Carbon nanotubes were rediscovered many times after that.

In 1966, Robert Young suggested the use of piezomotors for positioning; these are currently used to move the tip in scanning-tunneling microscopes (STMs) and atomic-force microscopes (AFMs) with an accuracy of $10^{-2}-10^{-3}$ nm.

In 1968, Alfred Cho and John Arthur developed the theoretical foundations of nanotechnology for the processing of surfaces.

In 1974, the Japanese physicist Norio Taniguchi in his report "On the basic concept of nanotechnology" coined the term "nanotechnology," which he suggested using to name all the processes which take place in objects of size less than 1 μm.

In 1981, Gerd Binnig and Heinrich Röhrer developed their first STM, which enabled them to see individual atoms.

In 1985, Robert Curl, Harold Kroto, and Richard Smalley discovered fullerene – a molecule that resembles a soccer ball and contains 60 carbon atoms. This discovery accelerated the development of the fabrication technology of other carbon nanomaterials such as carbon nanotubes.

In 1986, the atomic-force microscope was introduced by Gerd Binnig, Calvin Quate, and Christoph Gerber. The same year the book *Engines of Creation*, by Eric Drexler which has been called the Bible of nanoscience, was published. Eric Drexler described in his book molecular self-replicating robots, which can assemble molecules, decompose molecules, record in a nanocomputer's memory programs for self-replication, and realize these programs. The predictions for a 20-year period made in this book are incredibly becoming reality. Also in 1986, the American physicist Arthur Ashkin invented *optical tweezers* – the device for manipulation of microobjects and nanoobjects with the help of a focussed laser beam.

In 1987, the French physicist Jean-Marie Lehn introduced the notions of "self-organization" and "self-assembly."

In 1990, Donald Eigler showed that it is possible to develop a molecular automaton. With the help of STM he wrote on one of the crystallographic edges of nickel the name of his company "IBM" using 35 individual xenon atoms.

Further studies showed that it is possible to fix atoms to the surfaces of other materials. Submolecular assembly became a reality from this moment on.

In 1991, the first artificial metamaterial, which was called by its creator, the American physicist Eli Yablonovich, "photonic crystal," was produced.

In 1998, the Dutch physicist Cees Dekker fabricated the first field-effect nanotransistor, which was based on a carbon nanotube. The technology for fabrication of nanotubes of length larger than 300 nm was developed.

In 1999, the American physicists Mark Reed and James Tour formulated the principles of the manipulation of a single molecule as well as chains of molecules.

In 2000, the principles of nanotomography, i.e., the creation of three-dimensional images of the inner structure of matter with a resolution of 100 nm, were developed.

In 2001, IBM researchers developed the first examples of logical circuits constructed on the basis of carbon-nanotube field-effect transistors.

In 2002, Cees Dekker created the first bionanostructure – a synthesis of a carbon nanotube and a DNA molecule.

In 2003, an international team of researchers deciphered the sequence of the human genome.

In 2004, British and Russian scientists obtained the first samples of graphene – a single layer of graphite, which has a two-dimensional hexagonal lattice.

In 2001–2005 a team of American scientists deciphered the mechanism of the replication of genetic information by cells.

In 2007 an international group of physicists from the USA, Germany, and Holland developed a scanning-electron microscope with subatomic resolution of 0.05 nm. The same year a group of American scientists developed the technology of scanning nanolithography with a resolution of 12 nm and a recording speed of more than 1 mm s^{-1}.

At present it is commonly accepted that Nobel laureate Richard Feynman in his lecture "There's plenty of room at the bottom" was the first to relate nanostructures and nanotechnology. In his lecture Feynman suggested that in the future it will be possible to move individual atoms with the help of devices of the same size. Using such devices, macroobjects can be assembled atom by atom, making the fabrication process cheaper by several orders of magnitude. It will be enough to supply these nanorobots with the necessary amount of molecules and write a program for the fabrication of the required product. In his lecture Feynman also mentioned the prospects of nanochemistry for the synthesis of new materials. As soon as physicists create these devices, which will be able to operate with individual atoms, most of the traditional methods of chemical synthesis will be replaced by the methods of atomic assembly. The development of such a technology at the atomic scale will help to solve many problems of chemistry and biology. One can only wonder how the great scientist envisioned the enormous potential of nanotechnology.