Министерство науки и высшего образования Российской Федерации
НАЦИОНАЛЬНЫЙ ИССЛЕДОВАТЕЛЬСКИЙ
ТОМСКИЙ ГОСУДАРСТВЕННЫЙ УНИВЕРСИТЕТ (НИ ТГУ)

Механико-математический факультет

УТВЕРЖДАЮ:
Декан ММФ ТГУ

Л. В.Гензе

Рабочая программа дисциплины

# Математическое моделирование наноструктурных материалов

по направлению подготовки
**01.04.01 Математика**

Направленность (профиль) подготовки :
**Математический анализ и моделирование (Mathematical Analysis and Modelling)**

Форма обучения
**Очная**

Квалификация
**Магистр**

Год приема
**2023, 2024**

СОГЛАСОВАНО:
Руководители ОП
А.В.Старченко

Председатель УМК
Е.А. Тарасов

Томск – 2023

**1. Course goal and competences.**

The mail goal of this course is a study of general concepts and terms of molecular physics and nanomaterials modeling, models (numerical, physical and mathematical) for constructing new types of nanomaterials or for describing interaction of nanostructures with molecules or atoms.

**PC-1** Able to independently solve research problems of a scientific (scientific, technical, innovative) project

IPC-1.1 Able to do research aimed at solving individual research problems

IPC-1.2 determines the ways of practical use of scientific (scientific and technical) results

IPC-1.3 provides mentoring in the research process

**2. Course Aims**

- Develop a strong understanding of nanostructures models creation and application (ER-1)
- Learn about actual applications of molecular physics and nanostructures modeling (ER-2)
- Prepare concept of knowledge translation for low skilled or fresh colleagues (ER-3)

**3. Course place and impact in the curriculum**

This course is a one of the courses of Professional cycle, selective course in block 1 of elective part of education program.

Nanostructures material modeling is a basic course for master students who chose specialization on scientific topics of Theoretical Mechanics Department. It is a fundamental base for research project work in student's research practical training.

**4. Semesters and type of final assessment**

The First semester, type of final assessment – exam

**5.** ***Course prerequisites***

None

**6. Language of instruction**

English

**7. Course structure and types of learning activities**

6 ECTS and 216 hours

| | |
|---|---|
| Lectures | 32 |
| Practices | 32 |
| Consultation | 3,2 |
| Exam | 4,3 |
| Self-study work (SSW): | 130,8+13,7 |
| Exam preparation | 13,7 |

**8. Course content**

***Chapter 1 Molecular Physics and nanostructures***

1.1 Methods and ideas for many particles systems

1.2 Molecular system condition, law of equiprobability and ergodic hypothesis
1.3 Probability of macro condition
1.4 Fluctuations. Canonical ensemble
1.5 Maxwell distribution
1.6 Boltzmann distribution. Pressure
1.7 Temperature. Laws of thermodynamics
1.8 Processes in ideal gases. Heat capacity. Entropy
1.9 The Second law of thermodynamics. Thermodynamics functions
1.10 Interaction forces. Van der Waals equation
1.11 Joule–Thomson effect. Surface tension, evaporation and boiling
1.12 Liquid solutions. Chemical potential and phase rule
1.13 Kinematic characteristics of molecular movement. Transfer processes in gas media
1.14 Physical effects in low-density gases
1.15 Transfer processes in liquid media

***Chapter 2 Mathematical models of nanomechanics and nanostructures***

2.1 Nanoparticles in animate and inanimate nature
2.2 Nanoporus materials and its interaction with molecules
2.3 Movement of matter through nanoporus membranes
2.4 Intermolecular pair potentials
2.5 Continual and discrete ideas of intermolecular interaction of nanostructures
2.6 Features of realization numerical models of nanoobjects interaction with different atoms and molecules

## 9. Students' progress active monitoring

During the implementation of the course, classical educational technologies are used – lectures, practical classes, and independent study of materials by students, testing knowledge through tests, colloquia and exams. To conduct ongoing monitoring of the SSW, the teacher can conduct small tests at the beginning of each lesson.

The questions of the colloquia and the exam are a generalization of the questions of the current control tests and allow assessing the level of competence formation and understanding of the formation of the physical picture within these sections.

## 10. Course guideline for students and exam policy

For the successful mastering of the material, students need to use the sources, information systems and databases that are presented in the list of references. Independent work of students consists in the study of lecture material, material from practical classes and independent study of additional issues, a deeper analysis of lectures with the help of additional literature. Students should be attentive to the preparation for colloquia and exams, take a responsible approach to independent work and confidently answer the questions of current control tests.

Final assessment will be carried out by holding two colloquia (for each section of the discipline); the results of the colloquium will affect the assessment in the exam.

The exam can be scored a maximum of 5 points for each question. The final grade is summed up from the grades for each question and the grades for additional questions at the request of the teacher. Below is the formula for calculating the final grade:

$$S = \frac{S_1 + S_2}{2} + 0.2 * \sum_{i=1}^{n} d_i / n,$$

where S is the final grade for the test, $S_1$ and $S_2$ points for answers to the first and second questions, n is the number of additional questions, di is the points for the i-th additional question. The final grade is rounded in favor of the student if the fraction value exceeds 0.5. When answering a question, the completeness and accuracy of the answer, the logic and reasoning of the presentation of the material, the ability to use factual material in the answer are evaluated.

When answering the questions of colloquia and tests, the completeness and accuracy of the answer, the logic and reasoning of the presentation of the material, the ability to use factual material in the answer are evaluated. To set the current progress when monitoring the SSW, it is recommended to use the following table.

| Evaluation of the results of control of the SSW | Criteria |
|---|---|
| (Great) | The correct and detailed answer to the question is given. The student clearly and logically stated his answer to the question posed in the test. |
| (Good) | The correct answer to the question is given, but not everything is presented in detail and logically structured. |
| (Satisfactory) | In general, the correct answer to the question is given, but it is stated superficially and in violation of the logic of presentation. |
| (Unsatisfactory) | The answer is presented very superficially and in violation of the logic of presentation. The student has a very poor command of the basic models and concepts. Significant terminological and factual errors were made. |
| | An incorrect answer was given, a clear misunderstanding of the question in the test. |

## Sample list of questions for test and colloquia

1. What are fluctuations of physical quantities
2. What is entropy
3. Formulate the meaning of the Maxwell distribution over the velocities of molecules
4. Formulate the first law of thermodynamics
5. Formulate the second law of thermodynamics
6. Formulate the third law of thermodynamics
7. Van der Waals forces
8. What is surface tension
9. What is an isobar
10. What is an isotherm
11. Kihara's Potential
12. 13 Buckingham Potential
13. 14. Morse potential
14. 15. Peschl-Teller potential
15. 16. Continuum model of nanostructure representation
16. 17. Discrete model of nanostructure representation
17. 19. Hybridization of electron shells
18. 20. What are liquid membranes

## Sample list of questions for exam

1. Two-parameter potentials of pair molecular interactions
2. Polarization of a molecule
3. Multiparameter potentials
4. Ionization of a molecule
5. Monokinetic approximation of a molecular medium
6. Main tasks of molecular statistics
7. Maxwell distribution
8. Interaction of molecules with a spherical nanoparticle
9. Temperature of the gas medium
10. Temperature in crystal networks

11. Frequency spectrum of a graphene ring
12. Linearly independent modes of vibrations of graphene fragments
13. Energy transfer from molecules to graphene structure
14. Knudsen number
15. Discharged gaseous medium
16. Heat transfer of rarefied gas
17. Mobility of molecules
18. Diffusion of molecules in a gaseous medium
19. Brownian motion
20. Movement of protons in metals
21. Interaction of a xenon particle with surfaces
22. Xenon thermophoresis
23. Xenon centrifugation
24. Potential of intermolecular interaction
25. Interaction potential of high-molecular carbon with simple molecules
26. Smoothed energy of surface crystals
27. Packing density of carbon atoms in graphene sheets
28. Energy of interaction "nanoparticle - molecule"
29. Orbital motions of molecules around a spherical nanoparticle
30. Sorption molecules
31. Impact energy from an infinite nanothread
32. Modification of the Lennard-Jones potential
33. Nanotube resistance
34. Interaction of two fullerene particles
35. Surface carbon crystals

## 11. Education technologies and methodical support for course realization

a) Online course on TSU LMS platform «IDo» - https://lms.tsu.ru/course/view.php?id=6396

б) Tests and exam materials for this course (https://www.tsu.ru/sveden/education/eduop/).

## 12. Course literature and resourses

***a) Primary course literature.***

1. Kohanoff, Jorge, and Nikitas Gidopoulos. “Density functional theory: basics, new trends and applications.” Chapter 26 in Handbook of Molecular Physics and Quantum Chemistry. Edited by S. Wilson. Vol. 2, part 5. New York, NY: Wiley and Sons, 2003.
2. Ian Torrens, Interatomic Potentials, Academic Press (1972)
3. Many-Atom Interactions in Solids” ed. R.M. Nieminen, M.J. Puska and M.J. Manninen, Springer-Verlag, Proceedings in Physics Vol 48 (1990)

***b) Additional course literature.***

4. Peter J. F. Harris. Carbon nanotubes and related structures: new materials for the 21st century / Cambridge University Press, UK, 1999, 335 pp.
5. Tadashi Uragami. Science and Technology of Separation Membranes / John Wiley & Sons (WILEY), UK, 2017, 833 pp.
6. Chen, Gang. Nanoscale Energy Transport and Conversion: A Parallel Treatment of Electrons, Molecules, Phonons, and Photons. Oxford University Press, 2005.

***c) Databases and information and reference systems***

- http://e-science.sources.ru/

- http://www.coursera.org/
- https://ocw.mit.edu/index.htm

**13. Software list and internet resourses**
Microsoft Windows 7, Microsoft Windows 10
Microsoft Office 2010
Microsoft Visual Studio 2015, Intel Fortran/C/C++ Compiler 15
Mathcad 15, Maple 15, Matlab R2015;

Resourses:
– TSU library E-catalog – http://chamo.lib.tsu.ru/search/query?locale=ru&theme=system
– TSU E-library – http://vital.lib.tsu.ru/vital/access/manager/Index
– http://e.lanbook.com/
– http://www.studentlibrary.ru/
– https://urait.ru/
– https://znanium.com/
– http://www.iprbookshop.ru/

**14. Education and technical equipment**

Classical audiences with a whiteboard, a projector and a computer with a pre-installed Microsoft Office 2010 office suite will use for lectures. Classrooms 314, 316, 319 will use for practical classes and independent work of students.

№№314, 316
PC (13 шт.)
- LCD monitor BENQ 21.5”
- CPU Intel core i5-2400, 3.40 GHz
- RAM: 4 GB
- HDD 500 GB
- Nvidia GTS 450

№ 319
PC: (13 шт.)
- Monitor LG 24"
- CPU Intel Core i7-4790 3.60GHz
- RAM 16 GB
- HDD 1 TB

**15. Teaching staff**
Associate professor, PhD, Egor Tarasov
Assistant professor Anna Chelnokova
Assistant professor Valentina Poteriaeva