MINISTRY OF SCIENCE AND HIGHER EDUCATION OF THE RUSSIAN FEDERATION
Federal State Autonomous Educational Institution of
Higher Education
"Ural Federal University named after the First President of Russia B.N. Yeltsin"

Institute of Natural Sciences and Mathematics

APPROVED BY
Vice-Rector for Research
_____ A.V. Germanenko
«___» _____ 2023

PROGRAM OF THE DISCIPLINE
Solid State Chemistry

List of information about the postgraduate program	Credentials
Postgraduate program Solid State Chemistry	**Code PP** 1.4.15.
Group of scientific specialties Chemical Sciences	**Code** 1.4.
Federal State requirements (FSR)	Order of the Ministry of Science and Higher Education of the Russian Federation No. 951 dated 20.10.2021
Independently approved requirements (IAR)	The order "On the introduction of "Requirements for the development and implementation of training programs for scientific and scientific-pedagogical personnel in UrFU postgraduate school" № 315/03 dated 03.31.2022.

Yekaterinburg
2023

Program was compiled by the authors:

№ п/п	Name	Degree, Academic Title	Position	Affiliation
1	Cherepanov Vladimir Alexandrovich	Dr. Sci., Professor	Head of the Department.	Department of Physical and Inorganic Chemistry, Ural Federal University
2	Zuev Andrey Yurievich	Dr. Sci., Professor	Professor	Department of Physical and Inorganic Chemistry, Ural Federal University
3	Animitsa Irina Evgenievna	Dr. Sci., Assistant Professor	Professor	Department of Physical and Inorganic Chemistry, Ural Federal University

Recommended by:

Educational and methodological board of Institute of Natural Sciences and Mathematics

Head of the Educational and Methodological board of the Institute of Natural Sciences and Mathematics
Record № _1_ от 19.01.2023 г.

E. S. Buyanova

Agreed by:

Head of academic staff training department

E.A. Butrina

1.1.GENERAL CHARACTERISTICS OF THE DISCIPLINE OF SOLID STATE CHEMISTRY

1.2. Annotation of the content of the discipline

The special discipline "Solid State Chemistry" contributes to the development of basic professional competencies and their components and is aimed at an in-depth study of the basic sections of solid state chemistry: the fundamentals of the crystalline and electronic structure of solids, their reactivity, methods of synthesis and research.

1.2. The language of the discipline - English

1.3. Planned learning outcomes in the discipline

As a result of mastering the discipline, PhD student should gain:

knowledge:

- features of the crystalline state of matter;
- fundamentals of the electronic structure of solids;
- principles for obtaining materials with a functional characteristics;
- the relationship between the crystalline and defect structures of solids;
- thermodynamic aspects of the solids;
- features of methods for the synthesis of solids;
- basic physical and chemical methods for studying the functional properties of solid-phase inorganic materials

skills:

- to analyze data based on research;
- to develop an optimal scheme for obtaining crystalline materials or thin films, taking into account the required functional characteristics, structural and thermodynamic features of the material*;*
- to analyze the scientific literature on the topic of research, formulate the tasks of the work based on the analysis of the literature;
- to choose or independently create a methodology for the study of new material;
- to use specialized software and modern information technologies;
- to systematize the obtained theoretical and experimental data, generalize the knowledge gained and present the results obtained in the form of scientific publications;

mastering (to demonstrate skills and experience)

- the system of fundamental chemical concepts;
- the thermodynamic approach to the description and study of the solid state;
- the methodology for studying the structural and thermodynamic features of a material;
- the skills of modeling the main research processes;
- the skills of working with scientific literature and databases in order to determine the direction of research and solve specialized problems;
- science communication skills;
- the skills of choosing research methods, including the study of the physicochemical properties of substances in the crystalline state;
- the principles of organizing an experiment to obtain and study the functional properties of simple and complex oxides;

1.4. Content of the discipline

№ п/п	Types of educational work	Volume of discipline		Distribution of the volume of discipline by semester (hours)
		Total hours	Incl. contact work (hours)*	6
1.	**Auditory lessons**	**4**	**4**	**4**
2.	Lectures	4	4	4
3.	Practical classes	0	0	0
4.	Unaided work of graduate students, including all types of current certification	**104**	**1**	**104**
5.	Interim attestation	**Exam**	**1**	**Exam, 18**
6.	**Total volume according to the curriculum, hours.**	**108**	**5**	**108**
7.	**Total volume according to the curriculum, z.u.**	**3**		3

2. CONTENT OF THE DISCIPLINE

section number	Section, topic of discipline *	Content
1	**Introduction.** *Lectures 1 hour;* *Individual work of a postgraduate student, 1 hour.*	Specificity of solid state chemistry as a branch of chemical science. General differences in the structure and properties of solids from gases and liquids. Classification of solids. Crystalline solids. Monocrystalline, polycrystalline and nanocrystalline states of solids. Single-phase and heterophase crystalline solids.
2	**The structure of solids.** *Lectures 1 hour;* *Individual work of a postgraduate student, 18 h.*	Topic 1. The structure of crystalline solids. The concept of the symmetry of the crystal lattice. Crystallographic space groups of symmetry. Categories of symmetry. Syngonia. Choice and types of elementary cells. molecular crystals. Crystals with ionic and covalent lattices. Pauling rules. Sizes of atoms or ions. coordination numbers. Topic 2. Ways of organizing structures. Structures with hexagonal and cubic close packing. Tetragonal packing. Packaging defects, polytypism. Polyhedral description of crystal structures. Isomorphism. Topic 3. Solid solutions of substitution, insertion and subtraction. Isovalent and heterovalent substitution, non-stoichiometric compounds. Topic 4. Types of chemical bonds in solids. Van der Waals interaction in molecular crystals, clathrates. Ionic model of crystal structure, Madelung constant, ionic lattice energy. Born-Haber cycle and thermochemical calculations. Topic 5. Fundamentals of the theory of the crystal field and the field of ligands as applied to solids. Influence of d-electrons. Energy of stabilization by the crystal field and cationic distribution. The Jahn-Teller effect. Comparison of tetrahedral and octahedral environments. Effect of unshared electron pairs. Band structure of crystals.

		Formation of zones as a result of overlapping orbitals. Fermi level. Chemical potential. General conception about methods for calculating the band structure of crystals.
3	**The real structure of crystals.** *Lectures 1 hour;* *Individual work of a postgraduate student, 24 h.*	Topic 1. Ideal and defect crystals. Types of defects. Electronic defects. Point defects. Thermodynamics of the formation of point defects. Defect formation and nonstoichiometry of crystals. Quasi-chemical model for describing the equilibrium of point defects. Interaction of point defects. Topic 2. Solids with structural disordering. Extended defects. Surface in the solids. Surface energy of a crystal. The role of the surface in the chemical reactions of solids. Topic 3. Mobility of point defects. Diffusion and self-diffusion in solids. Basic mechanisms of self-diffusion. Diffusion coefficient, diffusion activation energy. Diffusion due to concentration gradient, Fick's laws. Diffusion of point defects in an electric field. Nernst-Einstein equation. Methods for studying diffusion. The transport equation. Ionic and electronic conductivity in solids, the dependence on temperature and partial pressure of the volatile component. Mobility, transport numbers. Temperature dependence of ionic conductivity. Intrinsic and impurity conductivity. Superionic conductors (solid electrolytes). Topic 4. Measurement of conductivity at direct and alternating current with using electrochemical impedance method as a function of temperature, activities of oxygen and water vapor in the gas phase. Determination of carrier transport numbers by the EMF method (oxygen or water vapor galvanic cells). Determination of transport numbers by the Tubandt method. Oxygen permeability in oxide materials with mixed electron-ion conductivity. Measurement of thermo-EMF coefficients as a function of temperature and oxygen partial pressure. Topic 5. Extended defects. Crystallographic shear structures. Packing defects. Block boundaries and antiphase domains (boundaries), heterogeneous inclusions. Neutral and charged extended defects. Dislocations in crystals, main types. Causes of dislocation formation
4	**Phase transitions in solids.** *Lectures 1 hour;* *Individual work of a postgraduate student, 1 h.*	Thermodynamic classification of phase transitions. Stable and metastable phases. Representation of phase transitions on phase diagrams. Structural changes during phase transitions. Structure changes with increasing temperature and pressure.
5	**Chemical reactions of solids. Methods for obtaining solids.** *Individual work of a postgraduate student, 22 h.*	Topic 1. General regularitys of the rate of heterogeneous chemical processes with solids. Elementary kinetic stages of processes. The role of mass transpost. Processes limited by diffusion and kinetic stages. The role of nucleation in processes accompanied by the formation of solids. The main factors affecting the reactivity of solids. The role of impurities and defects. Chemical reactions on the surface. Methods for controlling the diffusion processes with solids. Non-thermal methods for increasing the reactivity of solids: photochemical, radiation-chemical, mechanical, etc.

		Topic 2. Solid-state synthesis. Thermodynamic regularities for the synthesis of solids. P-T-x phase diagrams of two-component systems as a geometric representation of thermodynamic data. Gibbs phase rule. Projections and sections of P-T-x diagrams. The main types of condensed phase diagrams of two-component systems: with a simple eutectic, with the formation of congruently and incongruently melting intermediate compounds, with separation in the liquid phase, with unlimited and limited solid solutions, with polymorphism of components and compounds. Condensed diagrams of ternary systems. Phase equilibria in the subsolidus region. Using phase diagrams to select synthesis conditions. Topic 3. Synthesis by solid-state reactions. Basic thermodynamic and kinetic laws. Experimental implementation, the role of temperature. Methods of intensification of solid-phase processes: dispersion of initial substances, methods of chemical homogenization. Coprecipitation of components from solutions. Cryochemical synthesis and spray drying. Crystallization from gels. Sol-gel process. Mechanochemical stimulation of solid-phase processes. Basic regularities and possibilities of mechanochemical processes. Self-developing high-temperature synthesis. Solid-state synthesis at high pressures.
6	**Solid State materials.** *Individual work of a postgraduate student, 20 h.*	Topic 1. Classification of solid-state materials according to functional properties. Ionic conductivity and solid electrolytes. Topic 2. Magnetic materials. Topic 3. Optical materials. Luminescent materials and phosphors. Topic 4. Superconducting materials. Areas and prospects of application.

3. ORGANIZATION OF PRACTICAL EXERCISES, INDIVIDUAL WORK

3.1. Practical exercises

not provided

3.2. Approximate topic of independent/unaided work

Chemical reactions of solids. Methods for obtaining solids. Solid State materials. The real structure of crystals.

3.2.1. An approximate list of topics for essays (essays, creative works)

not provided

3.2.2. Approximate topics of individual or group projects

not provided

4. FUND OF EVALUATION FACILITIES FOR CURRENT AND INTERIM ATTESTATION

4.1. EVALUATION CRITERIA

The criteria approved by the department are used to evaluate the achievements of graduate students for each control and evaluation event. The system of assessment criteria is based on three levels of mastering the components of competencies: threshold, advanced, high.

Competency components	Signs of the level of mastering the components of competencies		
	threshold	**advanced**	**high**
Knowledge	A graduate student demonstrates knowledge-acquaintance, knowledge-copy: recognizes objects, phenomena and concepts, finds differences in them, shows knowledge of sources of information, can independently reproduce actions on knowledge by independently reproducing and applying information.	A graduate student demonstrates analytical knowledge: he confidently reproduces and understands the acquired knowledge, assigns it to one or another classification group, independently systematizes it, establishes relationships between them, and applies it productively in familiar situations.	A graduate student can independently extract new knowledge from the outside world, creatively use it to make decisions in new and non-standard situations.
Skills	A graduate student is able to correctly perform prescribed actions according to an instruction, an algorithm in a known situation, independently performs actions to solve typical problems that require a choice from among known methods, in a predictably changing situation	A graduate student is able to independently perform actions (techniques, operations) to solve non-standard tasks that require a choice based on a combination of known methods in an unpredictably changing situation	A graduate student is able to independently perform actions related to solving research problems, demonstrates the creative use of skills (technologies)
Personal qualities	A graduate student has a low motivation for learning activities, shows an indifferent, irresponsible attitude to learning, assigned work	The graduate student has a pronounced motivation for learning activities, demonstrates a positive attitude towards learning and future work, and is active.	The graduate student has a developed motivation for educational and labor activity, shows perseverance and enthusiasm, diligence, independence, creative approach.

4.2. EVALUATION TOOLS FOR CURRENT AND INTERIM ATTESTATION

4.2.1. List of sample questions for the pass

not provided

4.2.2. List of sample questions for the examination.

1. Classification of solid-state materials - according to composition, structure, functional properties.
2. Structure of crystalline solids.
3. Types of chemical bonding in solids. Thermochemical calculations.
4. Thermodynamic classification of phase transitions. Stable and metastable phases.
5. Defects in crystals: classification, types, examples.
6. Quasi-chemical model for describing the equilibrium of point defects. Interaction of point defects.

Construction of Brower diagrams
7. Diffusion and self-diffusion in solids. Nernst-Einstein equation. Methods for studying diffusion.
8. Experimental methods for determining the nature and direction of mass transport in a solids (electrochemical method, modeling of interaction on a flat surface, method of radioactive tracers).
9. Ionic conductivity of solids.
10. Extended defects. Dislocations in crystals, main types.
11. Main factors affecting the reactivity of solids. The role of impurities and defects.
12. General laws of the rate of heterogeneous chemical processes involving solids. Elementary kinetic stages of processes.
13. Methods for managing the development of processes involving solids.
14. Ionic conductivity and solid electrolytes. Superionic conductors.
15. Magnetic materials. Functional parameters. Materials with the effect of giant (GMR) and colossal (CMR) magnetic resistance.
16. Optical materials. Luminescent materials and phosphors.
17. Superconducting materials. Areas and prospects of application.
18. Refractory materials. Composite materials, their classification and methodology of creation.

5. EDUCATIONAL-METHODOLOGICAL AND INFORMATION SUPPORT OF THE DISCIPLINE

5.1. Recommended literature.

5.1.1. The basic textbooks

1. Anthony R. West. Solid state chemistry and its applications; Second edition, student edition. Wiley: Blackwell, 2014; p 584. https://bajkulcollegeonlinestudy.in/StudyMaterialFinal/Chemistry/23%20GE-2T%20Solid-State-Chemistry-and-its-Applications-West-Anthony-R%20-%20Biman%20Ari.pdf
2. R.C. Ropp. Solid State Chemistry. Elsevier science: 2003; p. 541. https://mkimia.fst.unair.ac.id/wp-content/uploads/2018/04/Richard-C.-Ropp-Solid-State-Chemistry-2003.pdf

5.1.2. The additional литература

not provided

5.2. Teaching aids.

not provided

5.3. Software

1. Microsoft office (Word, Excel, Power point);
2. Adobe Reader X
3. ChemOffice 2010
4. Isis Draw (Version 2.5)
5. Mercury (Version 2.4.5)
6. AutoDock (Version 1.5)
7. MestReNova (Version 6.0.2)
8. Open Babel (Version 2.3.1)
9. Avogadro (Version 1.0.3)
10. RasMol (Version 2.7.5.2)
11. Jmol (Version 12.0.45)

5.4. Databases, information and reference and search systems

1. ScienceDirect: http://www.sciencedirect.com;
2. Web of Science: http://apps.webofknowledge.com;
3. Scopus: http://www.scopus.com;

4. Reaxys: http://reaxys.com;
5. SciFinder https://scifinder.cas.org
6. Espacenet https://ru.espacenet.com
7. RSCI https://www.elibrary.ru
8. EBSCO Discovery Service http://lib.urfu.ru/course/view.php?id=141; ;

5.5. Electronic educational resources

1. http://lib.urfu.ru;
2. http://lib.urfu.ru/course/view.php?id=76;
3. http://opac.urfu.ru;
4. http://lib.urfu.ru/mod/resource/view.php?id=2330;
5. http://lib.urfu.ru/course/view.php?id=75;
6. http://lib.urfu.ru/mod/data/view.php?id=1379.

6. LOGISTICS AND TECHNICAL SUPPORT OF THE DISCIPLINE

Information about the equipment of the discipline with specialized and laboratory equipment

Ural Federal University has special facilities for conducting lecture-type classes, seminar-type classes, group and individual consultations, current control and intermediate certification, as well as rooms for independent work and rooms for storage and preventive maintenance of equipment. Special rooms are equipped with specialized furniture and technical teaching aids that serve to present information to a large audience.

Ural Federal University has the material and technical support necessary for the implementation of the postgraduate program, the provision of disciplines (modules), research work and practices, in accordance with the requirements for the material, technical and educational and methodological support of the program orientation.