

## Chemistry & Materials Science

### Program outline

This document outlines the scope of themes that may be included in the Olympiad test. They are grouped by areas and followed by recommended references in English.

## The skill set of the winner of the Olympiad in Chemistry & Materials Sciences

### Analytical activities

The collection, processing, storing, systematization and analytical interpretation of information for acquiring qualitatively new knowledge and providing rationales for decision-making.

1. Fundamental knowledge. The winner of the Olympiad requires deep knowledge and understanding of basic sciences and interdisciplinary areas. They must:

know	be able to	possess the skill in
- the basics of chemistry, physics and mathematics; - the fundamentals of chemical thermodynamics theory, crystallography	- freely navigate in fundamental science	- applying theoretical knowledge to various problems

2. System analysis. The ability to analyze materials, processes and systems within broad interdisciplinary fields; to set and solve non-standard problems using appropriate analytical, computational and experimental methods, including innovative ones. The winner of the Olympiad must:

know	be able to	possess the skill in
- dominant trends in science; urgent research problems; latest advances in science and technology	- process large volumes of scientific information; work independently with various sources; - analyze the effectiveness of intermediate decisions; make changes to the work plan	- interpreting the results of model analyses in view of the capabilities and limitations of the employed methods

### Research activities

These activities are aimed at new knowledge and include fundamental and applied research.

1. Research. Ability to find and obtain necessary data on the research object, carry out a literature search, use databases and other information sources, model objects and processes and analyze the use of the latest technology. The Olympiad winner must:

know	be able to	possess the skill in
- the principles of modern methods for studying the composition, structure and properties of materials	- use scientific databases in the literature search; - process experimental results, including error analysis, interpret the findings and draw up research reports; - analyze and interpret the obtained results	- using computer technology to solve professional problems; - presenting the results of calculations and forecasts in graphical and analytical form

2. planning, organizing and processing the findings. The ability to plan and carry out experimental research, analyze and process the findings and draw conclusions. The Olympiad winner must:

know	be able to	possess the skill in
- methods for constructing and examining basic statistical indicators, processing and analyzing observation results	- make a plan of computational and experimental work	- working with statistical data; - choosing appropriate methods and research conditions

3. Communicative competencies. The ability to communicate with the general public and the professional community. The Olympiad winner must:

know	be able to	possess the skill in
- English (level B1 or above)	- express their thoughts correctly and logically in oral and written communication with the team	- academic writing

### Content

### Section 1. General and inorganic chemistry

1. Main types of chemical bonds. Representation of orbital hybridization. The geometry of polyatomic molecules
2. Acid-base balance. Solutions of strong electrolytes. Protolytic equilibrium in aqueous solutions of weak acids and bases
3. Heterogeneous equilibria in the system of solid state: solutions for insoluble electrolytes
4. Redox equation. Standard, real, and formal redox potentials. The direction and depth of a redox reaction
5. Chemistry of coordination compounds. Structure and isomerism of coordination compounds. Equilibria in solutions of coordination compounds
6. Chemistry of the elements. Typical valences, degrees of oxidation, resultant compounds, their physical and chemical properties, industrial applications

### Section 2. Physical chemistry

1. The first law of thermodynamics and its application. Internal energy, enthalpy. Heat capacity. The internal energy of a system. Heat and work. Equilibrium and non-equilibrium processes. Thermochemistry. Hess's law, the Kirchhoff equation
2. The second law of thermodynamics. Entropy. Thermodynamic potentials and characteristic functions. The Gibbs fundamental equation. Gibbs-Helmholtz equations. The third law of thermodynamics (the Nernst heat theorem), the Planck postulate. Chemical potential
3. Chemical equilibria. The law of mass action and the equilibrium constant. The isotherm equation, the isobaric and isochoric processes of a chemical reaction.
4. Phase equilibria. Heterogeneous systems. The Gibbs phase rule. The Clausius-Clapeyron equation. Phase diagrams. Properties of solutions
5. Thermodynamics of electrochemical systems. Electrochemical potential and equilibrium conditions. The EMF of an electrochemical cell, electrode potential. The Nernst equation. The electrical conductivity of electrolyte solutions. Ion mobility and transport numbers. The Debye-Hückel theory
6. Surface phenomena. Thermodynamics of surface phenomena. Adsorption. Gibbs and Langmuir's isotherm adsorption
7. Chemical kinetics and catalysis. Phenomenological kinetics. The effect of temperature on the reaction rate. The Arrhenius equation, activation energy, methods to determine activation energy
8. The fundamentals of statistical thermodynamics, the structure of matter. Quantum chemistry

### Section 3. Organic chemistry

1. The structure of organic molecules: the nature of the chemical bond, distribution of electron density in a molecule due to various electronic effects of its substituents, the geometric features of a molecule of organic matter, including all types of isomerism
2. The main classes of organic compounds: alkanes and cycloalkanes, alkenes, dienes, alkynes, aromatic hydrocarbons, halogen derivatives, alcohols, carbonyl compounds, carboxylic acids, nitro compounds, heterocyclic aromatic compounds, and heterofunctional compounds (hydroxycarbonyl, including carbohydrates, hydroxy and amino acids and others). The main methods of synthesis of all mentioned classes of compounds and their chemical transformations
3. Reaction mechanisms: the electronic and spatial structure of reagents and substrates
4. Natural sources of organic compounds, main methods for the synthesis of key substances, the transformation of these compounds into others by laboratory and industrial methods
5. The main practical applications of organic compounds
6. Interactions of organic substances with living organisms; the environmental aspects of organic chemical production
7. The basics of molecular spectroscopy (IR, UV, NMR), mass spectrometry and X-ray diffraction

#### Section 4. Solid-state chemistry

1. The structure of periodic crystals: basic principles. Symmetry elements and symmetry operations; the choice of a unit cell; point and space symmetry groups. Close-packed structures and coordination polyhedra in the crystal structure description. Polymorphism
2. Point defects in crystals. The relationship between the concentration of impurities and intrinsic point defects. The relationship between the concentration of point defects, nonstoichiometry and the environment of the sample. Diffusion and ionic conductivity
3. Extended defects: dislocations, disclinations and packing defects. The relationship between nonstoichiometry and the presence of extended defects. The interaction between point and extended defects.
4. Crystal growth. The dissolution-crystallization curve. The metastable crystallization zone. Supersaturation. The molecular kinetic theory of crystal growth. The Kossel-Stranski model. The Bravais law. The Wulff construction. Types of crystal growth. Epitaxial growth of crystals. Crystal twinning
5. Properties of solids and their relationship with the surface structure, the presence, type and concentration of defects and the size and shape of particles
6. The electronic structure of solids. Band theory. Metals, semiconductors and insulators. 1D and 2D metals and semiconductors. Electron and hole conductivity

#### Section 5. Materials science

1. Crystal structure, mechanical and physical properties of metals, ceramics and polymers. Characteristics of a microstructure of materials. The influence of crystallite size on the mechanical and physical properties of metals and ceramics. The Hall-Petch relationship. Strength (hardness) and plasticity. The crack resistance of ceramics
2. Functional materials. High-temperature materials. Nanocarbon materials: nanotubes, fullerenes, graphene. Composite materials: their structure and mechanical properties. Metal hardening mechanisms, combinations of hardening mechanisms in composites with metal matrices. The rule of mixtures in calculating the mechanical and physical characteristics of composites
3. Solid solutions: types and structures. Vegard's law for solid solutions. Alloys and intermetallic compounds. Phase transitions
4. Electrochemical current sources. A conductivity-based classification of materials. Temperature dependence of the electrical conductivity of metals, semiconductors, ionic and mixed conductors. Ionic conductors. The conductivity of heterogeneous systems. The measurement of ionic conductivity in solid electrolytes. Electrochemical impedance. Impedance spectroscopy
5. Stress-strain ( $\sigma$ - $\varepsilon$ ) curve for solids. Flow stress, yield stress and ultimate tensile strength
6. Fatigue of materials. Fatigue limit. The characteristics of the cyclic stress-strain response. A fatigue curve
7. Physical processes in the mechanical treatment of solids. Elastic and plastic deformation. Destruction. Local increases in temperature and pressure. Static electricity. Amorphization

## Recommended literature

### Section 1. General and inorganic chemistry

1. Fundamentals of terminology, reading, interpreting and solving problems in chemistry in English. General Chemistry. Advanced Level. Textbook / A. Fetisova, A. Svistunov, T. Litvinova; I.M. Sechenov First Moscow State Medical University. - Moscow, 2016.
2. Fundamentals of terminology, reading, interpreting and solving problems in chemistry in English. General Chemistry. Advanced Level. Workbook / A. Fetisova, A. Svistunov, T. Litvinova; I.M. Sechenov First Moscow State Medical University. - Moscow, 2016.
3. Fundamentals of terminology, reading, interpreting and solving problems in chemistry in English. General Chemistry. Advanced Level. Test book / A. Fetisova, A. Svistunov, T. Litvinova; I.M. Sechenov First Moscow State Medical University. - Moscow, 2016.
4. Garner W.E. Chemistry of the solid state. Butterworths Scientific Publications, 1955.

5. General Chemistry: Principles and Modern Applications / Ralph H. Petrucci, F. Geoffrey Herring, Jeffrey D. Madura, Carey Bissonnette. – 11th Edition. – Toronto : Pearson, 2017.; 28 cm. – ISBN 978-0-13-293128-1 .
6. Hoffmann R. Solids and surfaces: a chemist's view of bonding in extended structures. 1st edition. Wiley-VCH, 1989.
7. Lefrou C., Fabry P., Poignet J. C. Electrochemistry: the basics, with examples. – Springer Science & Business Media, 2012
8. N.N. Greenwood and A. Earnshaw. Chemistry of the elements. Butterworth-Heinemann, 1997.

### Section 2. Physical chemistry

1. Donald A. McQuarrie, John D. Simon: Physical Chemistry: A Molecular Approach. 1st edition, 1997.
2. Peter Atkins, Julio de Paula, James Keeler: Atkins' Physical Chemistry: Volume 1: Thermodynamics and Kinetics 11th Edition, 2018.
3. Ira N. Levine: Physical Chemistry. 6th Edition, 2008.
4. Boris S. Bokstein, Mikhail I. Mendeleev, David J. Srolovitz: Thermodynamics and Kinetics in Materials Science: A Short Course, 2008.
5. David W. Ball: Physical Chemistry 2nd Edition, 2014.

### Section 3. Organic chemistry

1. Clayden, Greeves, Warren Organic Chemistry, Oxford University Press, 2000.
2. Desiraju G.R. Organic solid state chemistry. Elsevier Science Ltd., 1987.
3. Hart H. "Organic Chemistry – A Short Course". Hart H., Habad C.M., Craine L.E., Hart D.J. – 13th edition. – Cengage Learning, 2011.
4. Smith, Michael B.; March, Jerry (2007), Advanced Organic Chemistry: Reactions, Mechanisms, and Structure (6th ed.), New York: Wiley-Interscience, ISBN 978-0-471-72091-1

### Section 4. Solid-state chemistry

1. John M. Cowley. Diffraction physics. 1975
2. Willmott P. An introduction to synchrotron radiation: techniques and applications. – John Wiley & Sons, 2019
3. Marc De Graef and Michael E. McHenry. Structure of Materials. An Introduction to Crystallography, Diffraction and Symmetry. Cambridge University Press, 2012
4. Hahn Th. (ed.) International tables for crystallography. Vol. A. Space-group symmetry. Published for the International union of crystallography, 2005
5. Appendix 1 Crystal Structure Descriptions, 2009
6. Pu Zhang A. To. Point group symmetry and deformation-induced symmetry breaking of superlattice materials. Published 2015

## Section 5. Materials science

1. Dennis W. Readey. Kinetics in Materials Science and Engineering. 2017
2. Richard M. Martin. Electronic Structure: Basic Theory and Practical Methods, 2015
3. T. W. Clyne D. Hull. An Introduction to Composite Materials, 2019
4. William D. Callister Jr., David G. Rethwisch, Materials Science and Engineering ,2014
5. Subir Kumar Bose and Sanat Kumar Roy , Principles of Metallurgical Thermodynamics ,2014
6. Stephen J. Pennycook , Peter D. Nellist Scanning Transmission Electron Microscopy: Imaging and Analysis, 2011
7. Ryan O'Hayre . Materials Kinetics Fundamentals. 2015
8. Emmanuel Craig. Nanomaterials: An Introduction to Properties, Synthesis and Applications. 2019
9. Zainul Huda. Metallurgy for Physicists and Engineers: Fundamentals, Applications, and Calculations. 2020
10. Satya Bir Singh, Alexander V. Vakhrushev , A. K. Haghi Materials Physics and Chemistry: Applied Mathematics and Chemo-Mechanical. 2021
11. Noam Eliaz, Eliezer Gileadi. Physical Electrochemistry: Fundamentals, Techniques, and Applications 2018

## Recommended online courses

### Section 1. General and inorganic chemistry

1. Fundamentals of General Chemistry <https://stepik.org/course/4859/promo>
2. Fundamentals of General Chemistry <https://sechenov.online/course?id=203>
3. [Advanced chemistry](https://www.coursera.org/learn/advanced-chemistry) <https://www.coursera.org/learn/advanced-chemistry>

### Section 2. Physical chemistry

1. Patrick J. O'Malley, Michael W. Anderson, Jonathan Agger: Introduction to Physical Chemistry. <https://www.coursera.org/learn/physical-chemistry#instructors>.
2. Christopher J. Cramer: Statistical Molecular Thermodynamics. <https://www.coursera.org/learn/statistical-thermodynamics>.
3. Rasul Abdullaev, Leonid Braginsky, Arthur Pogosov: Basics of thermodynamics. <https://www.coursera.org/learn/thermo-dynamics>.
4. Rafael Jaramillo, Jessica Sandland, John Harrold: Thermodynamics of Materials. <https://www.edx.org/course/thermodynamics-of-materials-2>.
5. Alberto Salleo: Thermodynamics and Phase Equilibria. <https://www.edx.org/course/thermodynamics-and-phase-equilibria>.

### Section 3. Organic chemistry

1. Organic chemistry - <https://sechenov.online/course?id=350>
2. Organic solar cells - <https://ru.coursera.org/learn/solar-cell>

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3. Organic Chemistry - New Organic Chemistry Playlist - YouTube
4. Crash Course Organic Chemistry - Crash Course Organic Chemistry Preview - YouTube
5. Alkanes & Alkenes | Organic Chemistry | FuseSchool - Alkanes & Alkenes | Organic Chemistry | FuseSchool - YouTube

#### Section 4. Solid-state chemistry

1. Transmission electron microscopy for materials science  
<https://www.coursera.org/learn/microscopy>
- 2.
3. Materials Science and Engineering: Crystallography  
<https://www.udemy.com/course/crystallography> (платный)
4. Fundamentals of Materials Science <https://www.coursera.org/learn/fundamentals-of-materials-science>
5. Microscopy: methods of visualisation in micro- and nano-scale  
<https://stepik.org/course/64582/promo>
6. Solid State - Chemistry. Crystallography <https://www.udemy.com/course/solid-state-chemistry/>

#### Section 5. Materials science

1. Semiconductor Manufacturing <https://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-780-semiconductor-manufacturing-spring-2003/syllabus/>
2. Electrical, Optical & Magnetic Materials and Devices  
<https://ocw.mit.edu/courses/materials-science-and-engineering/3-15-electrical-optical-magnetic-materials-and-devices-fall-2006/>
3. Electronic and Mechanical Properties of Materials  
<https://ocw.mit.edu/courses/materials-science-and-engineering/3-225-electronic-and-mechanical-properties-of-materials-fall-2007/>
4. Physics for Solid-State Applications <https://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-730-physics-for-solid-state-applications-spring-2003/>
5. Introduction to Nanoelectronics <https://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-701-introduction-to-nanoelectronics-spring-2010/>
6. Submicrometer and Nanometer Technology <https://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-781j-submicrometer-and-nanometer-technology-spring-2006/>
7. Nanotechnology: A Maker's Course  
<https://www.coursera.org/learn/nanotechnology>