Anastasiia Iosimovska
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Education:

2023 – present	**Skolkovo Institute of Science and Technology,** Materials Science Department, Master's program excellent academic performance, **GPA:** 5.0/5.0 to date
2023 – 2024	**Lomonosov Moscow State University** first year of a Master's program in Geology, Department of Crystallography and Crystal Chemistry
2019 – 2023	**Lomonosov Moscow State University,** Bachelor's Degree in Geology, Department of Crystallography and Crystal Chemistry, **GPA:** 4.74/5.0

Laboratory experience:

2024 – present	Industry Oriented Computational Discovery Laboratory, Skolkovo Institute of Science and Technology **Supervisor:** Alexander Kvashnin
	Project: "Adsorption Energies and Reaction Pathways of Ammonia Decomposition on WB Nanoparticles"
	- Conducting DFT calculations (VASP, ORCA) to investigate adsorption and reaction pathways. - Analyzing catalytic properties of W–B nanoparticles and assessing their potential applications. - Contributing to the preparation of a manuscript for publication.
2021 – 2024	Materials Discovery Laboratory, Skolkovo Institute of Science and Technology **Supervisor:** Artem Ogabov
	Project: "Thermodynamic Stability and Ionic Conductivity in Li/Na/K - Ge Binary System"
	- Predicted new phases in the Li/Na/K–Ge system using the USPEX evolutionary algorithm and performed DFT calculations (VASP) to evaluate their thermodynamic stability. - Contributed to the preparation of a manuscript for publication. - Results published in Journal of *Materials Chemistry A (2025), Applied Physics Letters.*
	Project: "Geochemical classification of elements"
	Led the project in full: defined objectives, developed methodology, performed data analysis, and visualized results.
2022 – 2023	Laboratory of New Materials for Solar Energy, Faculty of Materials Science, M.V. Lomonosov Moscow State University
	Project: "Theoretical assessment of chloride ion influence on grain growth of hybrid perovskites"
	- Developed an interatomic potential model for hybrid perovskites (ABX_3) and performed grain boundary stability calculations using GULP. - Analyzed the crystallochemical role of Cl^- ions in thin film formation and improved perovskite stability for solar cells. - Results published in *Mendeleev Communications (2024).*

<p align="center">Internships and educational practice:</p>

Artificial Intelligence Research Institute (AIRI)
Internship, 2025
Project: Machine-Learning Potentials for Accelerated Modeling of W–B Nanoparticles

<p align="center">Conferences:</p>

- **2025:** 67th All-Russian Scientific Conference at MIPT, Section on Modern Methods of Atomistic Modeling in Materials Science – Oral Presentation

- **2024:** 2nd Sino-Russian Symposium on Chemistry and Materials (2024) – **Best Poster Award**

- **2023:** Lomonosov Student Conference (2023) – **Oral Presentation On High-Pressure Chemistry**

- **2022:** Modern Trends in Computational Materials Discovery (21st USPEX workshop), Isfahan University of Technology (IUT), Isfahan, Iran – **Tutor And Poster Present**

  Day Of Scientific Creativity At The Moscow State University – **Winner's Certificate**

  All-Russian Annual Workshop On Experimental Mineralogy, Petrology And Geochemistry In Institute Of Geochemistry And Analytical Chemistry, Russian Academy Of Sciences, Moscow, Russia – **Poster**

<p align="center">Skills:</p>

Languages: Russian (native), English (Upper-Intermediate)
Modeling Methods:
- Crystal structure prediction (USPEX)
- Quantum-chemical calculations (DFT: VASP, Quantum ESPRESSO, FHI-aims, Gaussian, MOPAC, ORCA)
- Molecular dynamics (LAMMPS)
- Phonopy

Visualization: VESTA, OVITO, ChemCraft, Jmol, Avogadro
High-Performance Computing: Running and optimizing calculations on HPC clusters, writing scripts (Bash)
Programming & Data Analysis: Python
Documentation & Reporting: LaTeX, MS Office
Operating Systems: Linux, Windows

<p align="center">Publications:</p>

- Anastasiia V. Iosimovska, Alexey P. Maltsev, Ilya V. Chepkasov, Artem R. Oganov, "Thermodynamic Stability and Ionic Conductivity in Lithium-Germanium Binary System"

- Maltsev, A. P., Iosimovska, A. V., Chepkasov, I. V., & Oganov, A. R. (2025). Structure transformations and ionic conductivity in germanides of sodium and potassium. *Journal of Materials Chemistry A*.

- Marchenko, E. I., Belich, N. A., Iosimovska, A. V., Misyutin, V. A., Goodilin, E. A., & Tarasov, A. B. (2024). Theoretical assessment of chloride ion influence on grain growth of hybrid perovskites. *Mendeleev Communications*, *34*(3), 321-324.

- Chepkasov, I. V., Baidyshev, V. S., Iosimovska, A. V., Zamulin, I. S., & Kvashnin, A. G. (2025). Adsorption properties of crystalline and amorphous PdIr nanoparticles. A systematic first-principles study. *Journal of Catalysis*, *447*, 116102.

- Изучение природных клинкеров Восточной Монголии из комплекса Хамарин- Хурал-Хид, Йосимовска А.В., Чевычелов В.Ю. в сборнике XIII-я Всероссийская школа молодых ученых "Экспериментальная минералогия, петрология и геохимия": Сборник материалов, ИЭМ РАН, Черноголовка, с. 38-39