

# Maksim Grebeniuk

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Telegram

## SCIENTIFIC INTERESTS

**Materials Science and Chemistry:** crystal structure prediction, DFT, DFPT, molecular dynamics, superconductivity, machine learning, neural networks, solid-state physics, lattice dynamics, quantum chemistry, inorganic chemistry, coordination chemistry, physical chemistry, and electrochemistry.

## EDUCATION

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|--------------------------------------------------------------------------------------|----------------|
| <b>PhD in Materials Science and Engineering</b>                                      | 2026 - Present |
| Skolkovo Institute of Science and Technology (Skoltech), Moscow, Russia              | GPA: -/5.0     |
| Computational Materials Science                                                      |                |
| <b>Master's Degree in Materials Science</b>                                          | 2023 - 2025    |
| Skolkovo Institute of Science and Technology (Skoltech), Moscow, Russia              | GPA: 4.8/5.0   |
| Computational Materials Science                                                      |                |
| <b>Additional Professional Education</b>                                             | Jul. 2024      |
| M. V. Lomonosov Moscow State University (MSU), Moscow, Russia                        |                |
| Modern Methods of Quantum Chemistry and High-Performance Computing                   |                |
| <b>Bachelor's Degree in Chemistry</b>                                                | 2019 - 2023    |
| D. Mendeleev University of Chemical Technology of Russia (MUCTR), Moscow, Russia     | GPA: 4.36/5.0  |
| Skoltech Department "Organic and Hybrid Materials for Energy Conversion and Storage" |                |

## ACADEMIC EXPERIENCE

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| <b>Materials Discovery Laboratory, Skoltech, Moscow, Russia, Supervisor: Prof. Oganov A. R.   Research Intern</b>                                                                                                                          | Mar. 2024 - Present   |
| <ul style="list-style-type: none"><li>Crystal structure prediction and property investigation of ternary superconducting hydrides under high pressure conditions.</li></ul>                                                                |                       |
| <b>Southern University of Science and Technology (SUSTech), Shenzhen, Guangdong, China   Collaboration</b>                                                                                                                                 | Dec. 2025 - Present   |
| <ul style="list-style-type: none"><li>Crystal structure prediction of superconducting hydrides under high pressure conditions with MLIPs.</li></ul>                                                                                        |                       |
| <b>Laboratory for Industry-Oriented Computational Discovery, Skoltech, Moscow, Russia   Collaboration</b>                                                                                                                                  | Jan. 2025 - Present   |
| <ul style="list-style-type: none"><li>Direct prediction of the Eliashberg spectral function with Euclidean neural networks.</li></ul>                                                                                                      |                       |
| <b>Shenyang National Laboratory for Materials Science (SYNL), IMR CAS, Shenyang, China   Collaboration</b>                                                                                                                                 | Mar. 2024 - Present   |
| <ul style="list-style-type: none"><li>Crystal structure prediction and property investigation of ternary superconducting hydrides under ambient and high pressure conditions.</li></ul>                                                    |                       |
| <b>Materials Discovery Laboratory, Skoltech, Moscow, Russia, Supervisor: Prof. Oganov A. R.   Student</b>                                                                                                                                  | Dec. 2020 - Mar. 2024 |
| <ul style="list-style-type: none"><li>Crystal structure prediction and property analysis of ternary superconducting hydrides in the Ca–Y–H System using the evolutionary algorithm USPEX and quantum-chemical Methods.</li></ul>           |                       |
| <b>Department of Organic Chemistry, MUCTR, Russia, Moscow, Supervisor: Prof. Traven V. F.   Student</b>                                                                                                                                    | Feb. 2021 - Feb. 2022 |
| <ul style="list-style-type: none"><li>Synthesis and purification of 7-(diethylamino)coumarin derivatives via distillation, recrystallization, and chromatography; photophysical characterization by NMR and UV-Vis spectroscopy.</li></ul> |                       |
| <b>Center for Energy Science and Technology, Skoltech, Russia, Moscow, Supervisor: Prof. Troshin P. A.   Student</b>                                                                                                                       | Feb. 2020 - Jan. 2021 |
| <ul style="list-style-type: none"><li>Structural and electrochemical characterization of a redox-active 2D Cu-THQ MOF cathode material for potassium-ion batteries using XRD, NMR, and voltammetry.</li></ul>                              |                       |

## SKILLS

### Computational Materials Science:

- Crystal structure prediction: USPEX.
- Density functional theory (DFT) and Quantum chemistry: VASP, Quantum ESPRESSO, FHI-Aims, EPIq, Wannier90, Gaussian, MOPAC, ORCA.
- Machine Learning: Training MLIPs (Moment Tensor Potential) and fine-tuning GNNs (MatterSim Potential) for Crystal Structure Prediction, Lattice and Molecular dynamics simulations and property predictions.
- Lattice dynamics: Phonopy, The Stochastic Self-Consistent Harmonic Approximation (SSCHA).
- Molecular dynamics: LAMMPS.

### Experimental Chemistry:

- Organic and Metal-organic synthesis, distillation (atmospheric pressure and vacuum), Recrystallization, Chromatography.

### Languages:

- Russian (Native)

- English (Upper-intermediate)

#### AI-Assisted Development:

- Leveraged LLMs (QWEN, ChatGPT, DeepSeek, Perplexity, Gemini) for code prototyping, debugging, and documentation generation in Python and Bash workflows.

#### Other:

- Linux cluster user, High-performance computing, LaTeX, Python (visualization, data analysis), MS Office, ChemDraw, Jana2006, WinXPOW.

#### LIST OF PUBLICATIONS

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**Ternary superconducting hydrides in Ca–Y–H system** | *In work*

**High-pressure phase stability and superconductivity in La–Zr–H hydrides** | *Submitted, Paper in refereed journal* 2026

- Open access: <https://arxiv.org/abs/2603.11590>.

#### HONORS & AWARDS

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**The 5th Conference on Physics under Synergetic Extreme Conditions, Huairou, Beijing, China** | *Speaker* Jul. 2026

- Oral presentation: High-pressure Phase Stability and Superconductivity in La–Zr–H Hydrides.

**23<sup>rd</sup> online USPEX workshop, Moscow, Russia** | *Speaker* Nov. 2025

- Oral presentation: Prediction of new high-temperature superconductors with USPEX.

**The 6<sup>th</sup> international conference «Fundamental problems of superconductivity-2025», Moscow, Russia** | *Participant* Sep. 2025

- Oral presentation: Superconductivity in Ca–Y–H at high pressures.
- Oral presentation: Direct prediction of Eliashberg spectral function with Euclidean neural networks.

**XIII International Conference on Magnetic and Superconducting Materials, Yerevan, Armenia** | *Participant* Sep. 2025

- Poster session: Ternary Superconducting Hydrides in Ca–Y–H System.

**Conference "Matter and Materials", Skoltech, Moscow, Russia** | *Participant* Mar. 2025

- Poster session: Hot Superconductivity in CaYH<sub>18</sub> Structure at High-Pressure.

**XXII Mendeleev Congress on General and Applied Chemistry, Sirius federal territory, Sochi, Russia** | *Participant* Oct. 2024

- Poster session: High-temperature superconductivity in clathrate Ca–Y hydrides.

**School on Current Issues of Condensed Matter Physics “Advanced Quantum Materials”, Makhachkala, Russia** | *Lecturer* Sep. 2024

- Lecture 1: Crystal Structure Prediction.
- Lecture 2: Introduction to Lattice Dynamics and Anharmonicity.
- Lecture 3: Practical Guide: Predicting New Superconducting Structures.

**Conference "PhysChem Challenges 2024", «Kiyazma» resort, Moscow region, Russia** | *Participant* Jul. 2024

- Poster session: Possible room-temperature superconductivity in Ca–Y–H system at high pressure.

**2<sup>nd</sup> Sino-Russian Symposium on Chemistry and Materials, Skoltech, Moscow, Russia** | *Participant* Jun. 2024

- Poster session: High-temperature superconductivity in Ca–Y–H system.

**66 All-Russian Science Conference, MIPT, Dolgoprudny, Russia** | *Participant* Apr. 2024

- Topic: High-temperature superconductivity in Ca–Y–H system at high pressure.

**Online Intensive on Molecular Dynamics Methods and Machine Learning Potentials, MIPT-Skoltech, Moscow, Russia** | *Participant* Jan. 2024

- Analyzing the multicomponent AlHfNbTaTiZr alloy's thermodynamic stability using Monte Carlo method implemented in LAMMPS.

**VTB Bank personal grants for developing hard and soft skills, Moscow, Russia** | *Participant* Dec. 2023

**First All-Russian Conference on Computational Materials Science, Skoltech, Moscow, Russia** | *Participant* Nov. 2023

- Poster session: Ternary superconducting hydrides in Ca–Y–H system.

**65 All-Russian Science Conference to Commemorate L.D. Landau's 115th Birthday, MIPT, Dolgoprudny, Russia** | *Participant* Apr. 2023

- Topic: Ternary superconducting hydrides in Ca–Y–H system.

**XVII Conference of Young Scientists, Graduates and Students “PHYSICOCHEMISTRY - 2022”, IPCE RAS, Moscow, Russia** | *Participant* Dec. 2022

- Topic: Prediction of new high-temperature superconducting polyhydrides based on calcium and yttrium.

**MUCTR, Moscow, Russia** | *Participant* Apr. 2022

- **XIV International Scientific and Practical Conference Education and Science for Sustainable Development.**
- Topic: Superconductivity in binary and ternary hydrides under high pressure.