

# Maksim Grebeniuk

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## SCIENTIFIC INTERESTS

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**Materials Science and Chemistry:** Crystal structure prediction, DFT, Superconductivity, Solid-state physics, Quantum chemistry, Inorganic chemistry, Coordination chemistry, Physical chemistry, Electrochemistry.

## EDUCATION

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**Master's Degree in Materials Science** Expected July 2025  
Skolkovo Institute of Science and Technology (Skoltech), Moscow, Russia GPA: -/5.0  
Computational Materials Science

**Bachelor's Degree in Chemistry** 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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**Computational Materials Discovery Laboratory, Skoltech, Supervisor: Prof. Oganov A. R. | Student** Dec 2020 - Present

- Applied evolutionary algorithm USPEX and Quantum Chemistry methods for crystal structure prediction and studying properties of ternary superconducting hydrides in Ca-Y-H system.

**Department of Organic Chemistry, MUCTR, Supervisor: Prof. Traven V. F. | Student** Feb 2021 - Feb 2022

- Applied distillation, recrystallization, chromatography, NMR, spectrophotometry, UV-Vis methods for synthesis and studying the fluorescent properties of 7-(Diethylamino)-Coumarin derivatives.

**Center for Energy Science and Technology, Skoltech, Supervisor: Prof. Troshin P. A. | Student** Feb 2020 - Jan 2021

- Applied XRD, NMR, Voltammetry methods for studying the structure and electrochemical characteristics of a redox-active 2D Copper-Benzoquinoid Metal-Organic Framework (Cu-THQ MOF) as a cathode material for Potassium-ion batteries.

## HONORS & AWARDS

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**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** April 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** April 2022

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

## SKILLS

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### Computational Chemistry:

- Crystal structure prediction: USPEX.
- DFT: VASP, Quantum ESPRESSO, FHI-Aims, EPIq, Wannier90, Gaussian, MOPAC, ORCA.
- Phonon calculations: Phonopy, Python-SSCHA.
- Molecular Dynamics: LAMMPS.

### Experimental Chemistry:

- Organic and metal-organic synthesis, Distillation (atmospheric pressure and vacuum), Recrystallization, Chromatography.

### Languages:

- Russian (Native speaker)
- English (Intermediate)

### Other:

- Linux cluster user, High-performance computations, LaTeX, Python (visualisation and data analysis), MS Office, ChemDraw, Jana2006, WinXPOW.