Maksim Grebeniuk

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SCIENTIFIC INTERESTS

Materials Science and Chemistry: Crystal structure prediction, DFT, DFPT, superconductivity, solid-state physics, quantum chemistry, inorganic chemistry, coordination chemistry, physical chemistry, electrochemistry.

EDUCATION

Master's Degree in Materials Science Expected July 2025

Skolkovo Institute of Science and Technology (Skoltech), Moscow, Russia GPA: -/5.0

Computational Materials Science

Additional Professional Education July 2024

Lomonosov Moscow State University (MSU), Moscow, Russia

Modern Methods of Quantum Chemistry and High-Performance Computing

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

Computational Materials Discovery Laboratory, Skoltech, Supervisor: Prof. Oganov A. R. | *Research Intern* Mar. 2024 - Present

- Crystal structure prediction and investigating properties of ternary superconducting hydrides at high pressure.

Computational Materials Discovery Laboratory, Skoltech, Supervisor: Prof. Oganov A. R. | *Student* Dec. 2020 - Mar. 2024

- 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.

SKILLS

Computational Chemistry:

- Crystal structure prediction: USPEX.
- DFT: VASP, Quantum ESPRESSO, FHI-Aims, EPIq, Wannier90, Gaussian, MOPAC, ORCA.
- 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 speaker)
- English (Upper intermediate)

Other:

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

HONORS & AWARDS

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

- Poster session: Hot Superconductivity in $CaYH_{18}$ 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.

PhysChem Challenges 2024, «Klyazma» resort, Moscow region, Russia | *Participant* Jul. 2024

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

2nd 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.