Daniil Kargin

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Education

Nanyang Technological University, Singapore *Aug 2023 – present*
BS(Honours) in Chemistry and Biological Chemistry with minor in Mathematical Sciences

- GPA: 4.81/5.0, predicted Honours (Highest Distinction)
- College of Science Dean's List, AY 2024-2025
- **Coursework:** Organic Chemistry, Physical Chemistry, Analytical Chemistry, Computational Chemistry, Quantum Mechanics, Discrete Mathematics, Abstract Algebra

Riga Secondary School No.10, Riga, Latvia *Sep 2011 – May 2023*
Secondary diploma with focus in Physics, Mathematics and Chemistry

- GPA: 9.53/10
- Valedictorian, recipient of Latvian Finance Ministry Centenniary Excellence Scholarship

Achievements and Awards

NTU President Research Scholar 2024

Latvian Prime Minister Prize for outstanding results in the international Chemistry Olympiad 2024, 2023

Latvian Government Prize for achievements in international Olympiads 2023, 2022, 2021

Latvian Ministry of Finance Centenniary Excellence Scholarship 2023

International Chemistry Olympiad (IChO) silver medal 2023, 2021

International Chemistry Olympiad (IChO) bronze medal 2022

Chemistry Olympiad of the Baltic States gold medal 2023

Chemistry Olympiad of the Baltic States silver medal 2022

International Genius Olympiad Conference, New York (USA), Honourable Mention prize in Research section 2022

Latvian National Chemistry Olympiad, Riga (Latvia) gold medal 2023, 2022, 2021, 2020

Latvian National Student Research Competition , Riga (Latvia) - Gold medal in Chemistry section 2022

Professional Experience

Undergraduate Research Assistant *Singapore*
Nanyang Technological University Lu Yunpeng Group *July 2024 – present*

- URECA Research Scholar
- Designed and implemented high-performance numerical algorithms in FORTRAN and C++ for evaluating kinetic rate constants and electronic spectra using DVR methods
- Developed a machine learning data visualisation software package in Python and Mathematica
- Analyzed simulation results using Mathematica

Research Intern *Riga, Latvia*
Riga Technical University (RTU) Konrade lab *Sep 2022 - Jan 2023*

- Developed new fluorescent biological markers
- Experimentally quantified fluorescence properties of dye molecules
- Carried out high sensitivity analysis

Research Intern *Riga, Latvia*
Latvia Organic Synthesis Institute (LOSI) Grigorjeva lab *Sep 2021 - May 2022*

- Developed a catalysis procedure with 3-valent cobalt to yield potential anti-cancer drugs
- Worked in a team to produce an international award-winning research paper and successfully present it at an international conference in New York
- Substituted a palladium catalyst by a 200x cheaper cobalt catalyst with greater yields

Publications and Conference Proceedings

Cobalt-catalyzed amino acid C(sp^2)-H functionalization using organic isocyanides May 2022

Latvian Student Research Conference. Riga, Latvia, Gold Prize in Chemistry section

Cobalt-catalyzed amino acid C(sp^2)-H functionalization using organic isocyanides July 2022

Genius Olympiad Student Research Conference. New York, USA, Honourable Mention prize in Research section.

Theoretical problems from the Baltic Chemistry Olympiad: 1st-30th BChO from 1993 to 2024. April 2024

Päkk Andreas, Smošljajev Artemi, *Kargin Daniil*, Narvaišs Nauris, Ivanistsev Vladislav.
Tartu: Tartu University Press. ISBN 978-9916-27-520-7.

Projects

Multi-Dimensional Discrete-Variable Quantum Wavepacket Time Evolution Simulation *github/DVRsincbasis*

- Developed an algorithm to solve multi-dimensional "particle in a potential well" problem using discrete-ordinate methods with particle in a box basis functions for initial wavepacket propagation on potential energy surface
- Optimized computation efficiency due to approximate potential operator matrix diagonalisation
- Developed a data visualisation program in Mathematica
- Tools Used: FORTRAN, Mathematica

HVZ Project — Co-Founder *Placeholder*

- Collaborating on the project with Rostislavs Rostovskis, Latvia University Solid State Physics Institute and Yew Mun Yip, Francis Crick Institute
- The first known attempt to try to develop a commercially feasible non-plane wave fully *ab initio* MD algorithm for drug-design applications
- Team management, literature search, data analysis, troubleshooting
- Tools Used: Rust, FORTRAN, C++

Camp lecturer, Baltic Chemistry Olympiad *Website*

- Lectured Physical Chemistry to the national teams of Estonia and Latvia
- Worked in organising committee of an international-level competition
- Co-author of an anniversary book on Chemistry competition problems and history in the region

Skills

Programming Languages: C++, FORTRAN, Python, Mathematica, HTML

Languages: Russian, English, German, Spanish, Latvian

Data analysis and visualisation using machine learning algorithms and software packages

Quantum mechanics algorithm development, HPC programming, physical simulations using Gaussian, GROMACS

Teaching material design, lecture and tutorial delivery both individually and to large groups of students