Daniil Kargin

Singapore hi@kuravax.com 8463 7607 kuravax.com Kuravax

Education

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

- GPA: 4.86/5.0, predicted Honours (Highest Distinction)
- College of Science Dean's List, AY 24/25, 25/26
- Peer tutor, Division of Chemistry and Biological Chemistry, AY 24/25, 25/26

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

- Valedictorian, recipient of Latvian Finance Ministry Centenniary Excellence Scholarship

Achievements and Awards

NTU President Research Scholar 2025, 2024

NTU College of Science Dean's list award 2025, 2024

Latvian Prime Minister Prize for outstanding results in the international Chemistry Olympiad 2023, 2022, 2021

Latvian Ministry of Finance Centenniary Excellence Scholarship 2023

International Chemistry Olympiad (IChO) silver medal 2023, 2021

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 for Intel clusters in FORTRAN for optimised pseudospectral basis set quantum dynamics of chemical processes on covalent surfaces, with scalability to up to 64 MPI ranks
- Developed workflows for creating *ab initio*, symmetry-adapted potential energy surfaces using machine learning and neural networks
- Analyzed simulation results using Mathematica and Python

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

A Modern Discrete Variable Representation (DVR) Method of Solving the Time Dependent Schrodinger Quantum Chemical Reaction Dynamics Problem June 2025

International Conference on Undergraduate Research (ICUR) 2025, Singapore. Poster and panel presentation.

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.

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.

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.

Projects

HVZ Project

- Collaborating on the project with Rostislavs Rostovskis, Latvia University Solid State Physics Institute
- Molecular dynamics and ab initio method development
- Supervision of high school research under schools' Independent Research projects and mentorship

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: Modern Fortran, Legacy Fortran, C++ (basic), Bash, Python, Mathematica, HTML

Languages: Russian, English, German, Spanish (intermediate), Latvian, Mandarin (basic)

Numerical methods: Quantum mechanics and machine learning algorithm development, numerical stability validation and performance profiling, optimised numerical libraries (Intel MKL, GNU BLAS/LAPACK), own scalable tensor-product linear algebra schemes with MPI distributed memory

HPC development: *Intel OneAPI* HPC toolkit, HPC programming using MPI, OpenMP, CUDA; Linux operating systems and Linux HPC clusters with PBS

Computational chemistry tools for HPC: Gaussian, VASP, ORCA, PySCF

Experimental chemistry techniques: organic synthesis; compound purification; spectroscopic methods (NMR, IR, UV-vis); analytical techniques (fluorimetry, mass spectrometry, HPLC, GC-MS); compound characterisation

Data analysis and visualisation using machine learning algorithms and software packages

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