

# Daniil Kargin

📍 Singapore 📩 hi@kuravax.com ☎ 8463 7607 ⚡ kuravax.com 🌐 Kuravax

## Education

<b>Nanyang Technological University, Singapore</b> <i>B.Sc. (Honours) in Chemistry and Biological Chemistry with minor in Mathematical Sciences</i>	<i>Aug 2023 – present</i>
<ul style="list-style-type: none"><li>◦ GPA: 4.90/5.0, predicted Honours (Highest Distinction)</li><li>◦ College of Science Dean's List, AY 24/25, 25/26</li><li>◦ Peer tutor, Division of Chemistry and Biological Chemistry, AY 24/25, 25/26</li></ul>	

<b>Riga Secondary School No.10, Riga, Latvia</b> <i>Secondary diploma with focus in Physics, Mathematics and Chemistry</i>	<i>Sep 2011 – May 2023</i>
<ul style="list-style-type: none"><li>◦ Valedictorian, recipient of Latvian Finance Ministry Centennial Excellence Scholarship</li></ul>	

## Publications and Conference Proceedings

<b>An 8-dimensional symmetry-adapted neural network potential energy surface for H<sub>2</sub> dissociative chemisorption on hexagonal boron nitride ortho site with explicit surface atom motion</b> <i>Kargin Daniil, Lu Yunpeng. J. Chem. Phys. 164, 014303 (2026). doi: 10.1063/5.0309397</i>	<i>Jan 2026</i>
<b>A Modern Discrete Variable Representation (DVR) Method of Solving the Time Dependent Schrodinger Quantum Chemical Reaction Dynamics Problem</b> <i>International Conference on Undergraduate Research (ICUR) 2025, Singapore. Poster and panel presentation.</i>	<i>June 2025</i>
<b>Theoretical problems from the Baltic Chemistry Olympiad: 1st-30th BChO from 1993 to 2024.</b> <i>Päkk Andreas, Smošljajev Artemi, Kargin Daniil, Narvaiš Nauris, Ivanistsev Vladislav. Tartu: Tartu University Press. ISBN 978-9916-27-520-7.</i>	<i>April 2024</i>
<b>Cobalt-catalyzed amino acid C(sp<sup>2</sup>)-H functionalization using organic isocyanides</b> <i>Genius Olympiad Student Research Conference. New York, USA, Honourable Mention prize in Research section.</i>	<i>July 2022</i>
<b>Cobalt-catalyzed amino acid C(sp<sup>2</sup>)-H functionalization using organic isocyanides</b> <i>Latvian Student Research Conference. Riga, Latvia, Gold Prize in Chemistry section.</i>	<i>May 2022</i>

## Professional Experience

<b>Undergraduate Research Assistant</b> <i>Nanyang Technological University Lu Yunpeng lab</i>	<i>Singapore</i> <i>July 2024 – present</i>
<ul style="list-style-type: none"><li>◦ URECA Research Scholar</li><li>◦ Designed and implemented high-performance numerical algorithms for HPC clusters in Fortran for optimised pseudospectral basis set quantum dynamics of chemical processes on covalent surfaces, currently investigating algorithm scalability on NSCC Cray clusters for up to 1000 cores</li><li>◦ Developed workflows for creating <i>ab initio</i>, symmetry-adapted and physics-aware potential energy surfaces using machine learning and artificial neural networks</li></ul>	
<b>Research Intern</b> <i>Riga Technical University (RTU) Konrade lab</i>	<i>Riga, Latvia</i> <i>Sep 2022 - Jan 2023</i>

- Carried out high sensitivity analysis

### **Research Intern**

*Latvia Organic Synthesis Institute (LOSI) Grigorjeva lab*

*Riga, Latvia*

*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

### **Skills**

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**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

### **Achievements and Awards**

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**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 Centenary Excellence Scholarship** 2023

**International Chemistry Olympiad (IChO)** silver medal 2023, 2021

### **Projects**

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#### **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