

# Daniils Kargins

(Daniil Kargin)

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## Research Interests

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Scientific Computing, High-Performance Numerical Simulations, Control, Stability and Identifiability Theory, Partial Differential Equations, Interdisciplinary Physical Chemistry.

## Education

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

- GPA: 4.90/5.0, 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 Centenary Excellence Scholarship

## Professional Experience

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**Research Assistant** *Singapore*  
*Nanyang Technological University, School of Electrical and Electronics Engineering* *Dec 2025 – present*

- Co-supervised by Prof. Hung Dinh Nguyen and Dr. Petr Vorobev; electrochemical modeling of battery cells.
- Control theory analysis for parameter identifiability of physical PDE models in smart BMS.
- Developing custom pseudospectral CFD engines in Fortran for heat simulations within battery stacks.

**Research Assistant** *Singapore*  
*Nanyang Technological University, School of Chemistry, Chemical Engineering and Biotechnology* *July 2024 – present*

- URECA Research Scholar under Dr. Lu Yunpeng; HPC algorithms in Fortran for quantum dynamics on covalent surfaces.
- Optimizing pseudospectral basis set scalability on NSCC Cray clusters (up to 1000 cores).
- Developing *ab initio*, symmetry-adapted potential energy surfaces using ML/ANNs.

**R&D Intern** *Singapore*  
*Energy Research Institute @ NTU, Electrification, Power and Grids Centre* *May 2026 – July 2026*

- Computer modeling of grid-scale Battery Energy Storage Systems (BESS).
- Integrating classical physical models with AI/ML for system optimization.

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

- Developed new fluorescent biological markers; quantified fluorescence properties of dye molecules.
- Carried out high sensitivity analysis using spectroscopic methods.

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

- Developed cobalt-catalyzed procedure for potential anti-cancer drugs (200x cheaper than palladium).
- Collaborated on international award-winning research paper presented at Genius Olympiad Conference.

## Publications and Conference Proceedings

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**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** Jan 2026

*Kargin Daniil*, Lu Yunpeng. *J. Chem. Phys.* 164, 014303 (2026). doi: 10.1063/5.0309397

**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 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.

## Teaching and Academic Service

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- **ICHO Camp Lecturer:** 2023–2025. Physical Chemistry lecturer for Estonia and Latvia national teams.
- **NTU Peer Tutor:** Division of Chemistry and Biological Chemistry (AY 24/25–25/26). Tutorial design and delivery to large groups, as well as in private.

## Mentorship and Supervision

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- **Nesterovs, Nikita** (Co-supervised with Rostislavs Rostovskis, UL Institute of Solid State Physics):
  - Latvian Student Research Conference, April 2026 – National Finalist, Natural Sciences section.
  - Riga Regional Student Research Conference, March 2026 – Silver Prize, Physics and Astronomy section.

## Achievements and Awards

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<b>Citizenship of the Republic of Latvia for Special Meritorious Service for the Benefit of Latvia</b>	2025
<b>NTU President Research Scholar</b>	2025, 2024
<b>NTU College of Science Dean's List Award</b>	2025, 2024
<b>Latvian Prime Minister Prize</b> for outstanding results in the international Chemistry Olympiad	2023, 2022, 2021
<b>Latvian Ministry of Finance Centenary Excellence Scholarship</b>	2023
<b>International Chemistry Olympiad (ICHO)</b> silver medal	2023, 2021

## Skills

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**Programming:** Modern Fortran, Python, Bash, Mathematica, MATLAB, HTML, C++.

**HPC & Simulation:** Intel OneAPI, MPI/OpenMP, CUDA, Linux clusters, numerical methods.

**Computational Chemistry:** Gaussian, VASP, ORCA, PySCF, Quantum Dynamics, ML potentials.

**Experimental Techniques:** Organic synthesis; NMR, IR, UV-vis; fluorimetry, MS, HPLC, GC-MS.

**Languages:** Russian (Native), Latvian, English, German (All Fluent), Spanish (Intermediate), Mandarin (Basic).