# Daniil Kargin

 ♦ Singapore
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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)
- 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

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

### Achievements and Awards

NTU President Research Scholar	2024
<b>Latvian Prime Minister Prize</b> 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

 $NTU\ Singapore$ 

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
- o Developed a machine learning data visualisation software package in Python and Mathematica
- Analyzed simulation results using Mathematica

Research Intern

Riga, Latvia

Sep 2022 - Jan 2023

Riga Technical University (RTU) Konrade lab

o 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

- o 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

 ${\rm May}\ 2022$ 

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

# 1D Discrete-Ordinate Schrodinger Equation Numerical Solution Algorithm

github/DVRsincbasis **∠** 

- Developed an algorithm to solve one-dimensional "particle in a potential well" problem using discreteordinate methods with particle in a box basis functions (Chebyshev polynomials)
- o Optimized computation efficiency due to approximate potential operator matrix diagonalisation
- o Developed a data visualisation program in Mathematica
- o Tools Used: FORTRAN, Mathematica

### MD software with ab initio DFT potential calculation

Placeholder 🗹

- Collaborating on the project with Rostislavs Rostovskis, Latvia University Solid State Physics Institute and Yew Mun Yip, Francis Crick Institute
- The first attempt to try to develop a fully ab initio algorithm for molecular dynamics
- o Team management, literature search, data analysis
- o Tools Used: Rust, FORTRAN

### Camp lecturer, Baltic Chemistry Olympiad

Website 🗹

- o 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 GROMACS and Gaussian

Advanced problem solving, both independently and in groups

Collaboration, communication, public speaking and presentation

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