

Anton Morgunov

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EDUCATION

Yale University

Ph.D. Candidate in Theoretical and Computational Chemistry

Jan 2025 - Jun 2029

New Haven, CT

Yale University

Chemistry M.Sc. Grade average: Honors

Aug 2023 - Dec 2024

New Haven, CT

Massachusetts Institute of Technology

S.B. in Chemistry and Biology. Minor in CS. GPA 5.0. Phi Beta Kappa.

Sep 2018 - May 2023

(on leave AY2020-2021) Cambridge, MA

RESEARCH EXPERIENCE

Prof. Victor S. Batista Lab

Graduate Student (Dept. of Chemistry)

New Haven, CT

Nov 2023 - Present

- Leveraged property-based chemical space to devise a novel and 10x more computationally efficient active learning procedure for aligning generative models to user-specified objective functions.
- Developed a novel approach to end-to-end multistep retrosynthesis prediction that outperforms SOTA on route quality. Placed 2nd in the Standard Industries Challenge after testing on natural products of interest.
- Deployed ML models developed in the lab and built an intuitive Web UI to make them accessible to the general public.

Prof. Troy Van Voorhis Lab

Undergraduate Researcher (Dept. of Chemistry)

Cambridge, MA

Feb 2022 - May 2023

- Benchmarked the accuracy of Δ HF, Δ MP2, Δ CC methods and different extrapolation schemes at predicting core-electron binding energies (CEBEs) for C-, N-, O-, and F-based molecules.
- Presented a novel MP2-based composite extrapolation scheme that recovers gold standard CCSD-grade CEBE predictions with high fidelity (within 0.02 eV) at a fraction of the computational cost.
- Wrote Python/Shell (2k+ lines) scripts that automate submission of calculations, parsing of results, extrapolation to the complete basis set limit, and assessment of accuracy by comparison to experimental data. Streamlined data analysis and visualization by creating a single function call that recreates all figures and tables from the manuscript.

Prof. Ronald T. Raines Lab

Undergraduate Researcher (Dept. of Chemistry)

Cambridge, MA

Sep 2018 - Dec 2021

- Designed and performed synthesis of diazo-compounds for the bioreversible esterification of proteins. Employed reverse-phased chromatography, and characterized organic structures using ^1H , ^{13}C NMR, APCI/ESI MS, LC MS.
- Calculated TS structure corresponding to the concerted mechanism of esterification reaction with DFT calculations.

PUBLICATIONS

- [1] Y. Shee, **A. Morgunov**, H. Li, and V. S. Batista. "DirectMultiStep: Direct Route Generation for Multistep Retrosynthesis". In: *Journal of Chemical Information and Modeling* 0.0 (2025), null. DOI: 10.1021/acs.jcim.4c01982. *Y.S. and A.M. contributed equally. GitHub.
- [2] H. Li, Y. Shee, B. Allen, F. Maschietto, **A. Morgunov**, and V. Batista. "Kernel-elastic autoencoder for molecular design". In: *PNAS Nexus* 3.4 (Apr. 2024), pgae168. ISSN: 2752-6542. DOI: 10.1093/pnasnexus/pgae168.
- [3] **A. Morgunov**, H. K. Tran, O. R. Meitei, Y.-C. Chien, and T. Van Voorhis. "MP2-Based Composite Extrapolation Schemes Can Predict Core-Ionization Energies for First-Row Elements with Coupled-Cluster Level Accuracy". In: *The Journal of Physical Chemistry A* 128.33 (2024), pp. 6989–6998. DOI: 10.1021/acs.jpca.4c01606. GitHub.
- [4] G. W. Kyro, **A. Morgunov**, R. I. Brent, and V. S. Batista. "ChemSpaceAL: An Efficient Active Learning Methodology Applied to Protein-Specific Molecular Generation". In: *Journal of Chemical Information and Modeling* 64.3 (Feb. 2024), pp. 653–665. DOI: 10.1021/acs.jcim.3c01456. *all authors contributed equally. GitHub.

SKILLS

- **Languages:** Python, Shell, \LaTeX , HTML, CSS, TypeScript. **Natural Languages:** English (fluent), Russian (native).
- **Scientific Software:** ORCA, PySCF, Q-Chem, Gaussian, SLURM, RDKit, Plotly, Matplotlib, PyTorch, Pandas, NumPy.
- **WebDev:** PostgreSQL, Next.JS, React, Flask, SQLAlchemy, Docker, NGINX, AWS.
- **Tools:** Photoshop, Illustrator, InDesign, Sketch, Git, GitHub, Word, Excel, PowerPoint.
- **Experimental Techniques:** Organic synthesis, NMR, LC-MS, HPLC, Time-resolved spectroscopy.

MY PHILOSOPHY

I adhere to two core postulates: that objective truth exists and that it's discernible through the scientific method. I believe that human beings are ordained to pursue eudaimonia through contemplation and investigation of the Universe. I'm particularly interested in the mechanisms of life, and chemistry, in my view, stands as the central science that provides direct path to their understanding. I decided to focus on theoretical and computational chemistry tools because they allow to minimize the time between formulation and testing of the hypothesis. In my day-to-day work, I prefer first-principles thinking, which is both a strength and a weakness, as sometimes I could've saved time if I studied more literature first. Fortunately, I succeed in surrounding myself with amazing people who complement my shortcomings.

Many recognize the value of scientific research, which by its nature expands our boundaries of knowledge. Few recognize, however, that in this process the starting point is as important as the delta by which you advance. Without concerted efforts to preserve the known, its boundaries will recede just like the plasma membrane contracts under reduced osmotic pressure. The knowledge frontiers are preserved by a system of education; therefore, I contribute to educational initiatives that promote science and support those who strive to go beyond school curriculum.

WORK EXPERIENCE

Los Alamos National Laboratory

Graduate Research Assistant

Los Alamos, NM

Jul 2024 - Feb 2025

- Worked on modeling light matter interactions from first principles in T Division (Center for Nonlinear Studies)

LEADERSHIP EXPERIENCE

Beyond Curriculum Public Foundation

Co-Founder

Project Manager, Accountant, Co-Founder

Kazakhstan

Aug 2024 - Present

Apr 2020 - Aug 2024

- Co-founded the pioneering student-led non-profit dedicated to fostering STEM interest beyond standard curricula
- Gathered and managed a fully-remote team of volunteers peaking at 70 members. Coordinated the launch of the largest database of past olympiad problems (2,000,000 pageviews monthly) and results, providing evaluation of every olympiad on transparency, selectivity, and uniqueness of problem tasks. Unified separate subject communities into a single platform (500k pageviews & 50k visits monthly, 50+ DEU, 34% DAU/MAU).
- Managed all financial and internal documentation, ensuring legal compliance
- Raised \$3,000+ from 270+ individual donations and established an endowment to ensure long-term sustainability. Secured \$13,000 to fund the creation of a cycle of 33 inspiring articles on why chemistry, biology, physics, math, and robotics are beautiful and worth pursuing as a career. Distributed 1000 free copies among students from rural areas by collaborating with IQanat Foundation. Distributed extra 5000 copies among schools in all regions of Kazakhstan.
- Secured a \$24,000 US Federal Grant to develop a pioneering free robotics course. Filmed 57 video lessons (with Kazakh subtitles) on Arduino, 3D printing, Neural Networks, and Computer Vision bringing knowledge previously available only in English. Hosted 3 talks by robotics researchers from UMich and Cornell, published 6 articles raising awareness about career pathways in robotics, women in robotics, and socio-economic barriers to robotics.
- 150k+ visitors per month, 90% of silver and gold medalists of national chemistry olympiad have used our platform.

Community Manager, Writer

Feb 2019 - Apr 2020

- Disrupted the olympiad system by opening the chemistry community to the general public completely for free and thereby democratizing the knowledge that used to be known only among a select number of elite specialized schools.
- Coordinated the launch of similar communities in physics, biology, math, and geography. Launched recurrent Q&A sessions with top ex-olympians, invited guests from Harvard, MIT, KAIST, Moscow State University.

Peer Tutor

May 2017 - Feb 2019

- Founded an online community of NIS students for Chemistry Olympiad preparation, leveraging personal expertise to develop a detailed study framework and inspirational content. Provided direct tutoring to over 100 students, culminating in having 50% of the 2019 national team members having studied with this community.

Kazakhstan Chemistry Olympiads Association

Head Mentor, Chairman

Kazakhstan

Nov 2021 - Mar 2023

- Established a national association of problem authors and mentors to increase transparency of national team selection processes and administration of chemistry olympiads in Kazakhstan. Published 70+ pages of analytical reports on the organization of national olympiads and the performance of students. Ensured publication of all internal documents and minutes of meetings, establishing an unprecedented level of transparency.

Problem Author, National Team Mentor

Feb 2019 - Nov 2021

- Wrote and graded 70+ problems for all stages of national olympiads, taught 150+ hours of olympiad chemistry.

- Represented Kazakhstani delegation, translated problems and arbitrated on behalf of students at IChO 2019-2022.
- Revolutionized the operation of national olympiads by single-handedly managing a pioneering website that published problems, solutions, and live results of the final stage coupled with immediate email notifications to participants.

Popular Science Magazine "Kvazar"

Editor, Writer, Designer

Kazakhstan

Nov 2015 - Sep 2017

- Wrote 30+ articles and designed layout for 9 issues published online. Collaborated with 10+ invited authors.
- Invited as informational partners for 8000-strong science festivals in Russia (Quantum Technology Conference 2018, Robotics Expo 2017, Science Fest 2017). 11k+ unique visitors per month on the website as of Sep 2017.

TEACHING EXPERIENCE

- General Chemistry II (Spring 2024). Teaching Fellow. Yale. My Notes
- General Chemistry Laboratory (Fall 2023). Teaching Fellow. Yale
- Fundamentals of Programming in Python (Spring 2023). Undergraduate Teaching Assistant. MIT
- Fundamentals of Programming in Python (Fall 2022). Undergraduate Teaching Assistant. MIT
- Fundamentals of Programming in Python (Spring 2020). Undergraduate Teaching Assistant. MIT
- Differential Equations (Spring 2020). Undergraduate Teaching Assistant. MIT
- Multivariable Calculus (Fall 2019). Undergraduate Teaching Assistant. MIT

AWARDS

- Phi Beta Kappa. Xi Chapter. (2023)
- Academic Achievement Award. MIT Chemistry Department. (2023)
- El Maqtanyshy (Pride of the Nation). Nursultan Nazarbayev Foundation. (2020)
- El Maqtanyshy (Pride of the Nation). Nursultan Nazarbayev Foundation. (2019)
- The one who brings students to an Olympian peak. Ministry of Education and Science. (2019)
- Gold Medal (Ranked 10/297). International Chemistry Olympiad. (2017)
- Gold Medal (Ranked 8/120). International Mendeleev Olympiad. (2017)

SELECTED COURSEWORK

Red denotes courses taken at MIT, blue denotes courses taken at Yale.

Theoretical Chemistry

- [Chem566-567](#) Quantum Mechanics
- [Chem572-573](#) Statistical Mechanics
- [Phys506](#) Mathematical Methods of Physics
- [5.73](#) Quantum Chemistry (Graduate Course)
- [5.62](#) Statistical Mechanics
- [5.61](#) Intro to Quantum Mechanics
- [5.04](#) Chemical Applications of Group Theory
- [5.60](#) Thermodynamics and Kinetics

Computer Science

- [Cpsc580](#) Computer Vision
- [Cpsc583](#) Deep Learning on Graphs
- [6.3900\(6.036\)](#) Machine Learning
- [6.1210\(6.006\)](#) Algorithms
- [6.3700\(6.041\)](#) Probability
- [6.1200\(6.042\)](#) Mathematics for Computer Science
- [6.1010\(6.009\)](#) Fundamentals of Programming
- [6.100B\(6.0002\)](#) Data Science with Python

Economics

- [14.12](#) Economic Applications of Game Theory
- [14.13](#) Psychology and Economics
- [14.26](#) Organizational Economics
- [14.01/02](#) Micro & Macroeconomics

General STEM

- [5.08](#) Chemical Biology
- [5.07](#) Biological Chemistry
- [5.43](#) Physical Organic Chemistry
- [5.13](#) Organic Chemistry II
- [7.06](#) Cell Biology
- [7.03](#) Genetics
- [5.361](#) Expression & Purification of Enzymes
- [5.362](#) Kinetics of Enzyme Inhibition
- [5.382](#) Time & Frequency Resolved Spectroscopy
- [8.022](#) Math-intensive Electricity & Magnetism
- [18.03](#) Differential Equations
- [18.02](#) Multivariable Calculus

AUDITED COURSEWORK

- [Cpsc571](#) Trustworthy Deep Learning
- [Chem584](#) Quantum Computing
- [Cpsc558](#) Automated Decision Systems
- [Cpsc577](#) Natural Language Processing
- [Cpsc576](#) Advanced Computational Vision
- [Cpsc586](#) Probabilistic Machine Learning
- [Cpsc563](#) Algorithms for Convex Optimization
- [Cpsc567](#) Cryptography
- [Astr610](#) Theory of Galaxy Formation
- [Chem568](#) Advanced Quantum Mechanics
- [18.650](#) Fundamentals of Statistics
- [6.046\(6.1220\)](#) Algorithms II