# Roman Korol

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## Current Position

**University of Rochester**, Rochester, New York

Postdoctoral Fellow since September 2023

## Education

**California Institute of Technology**, Pasadena, California

Ph.D. in Theoretical Chemistry, 2018–2023

**University of Toronto**, Toronto, Canada

B.Sc. (Honours) in Chemistry with High Distinction, 2014–2018

## Fellowships and Awards

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|---|---|
| Steadman Award | 2024 |
| Student Leader Award | 2024 |
| Gray-Hill Award Lecture | 2023 |
| Patricia Beckman Graduate Fellowship | 2018 |
| Michael Rebryk Memorial Scholarship | 2018 |
| Ivan Szak Scholarship in Chemistry | 2018 |
| St. Michael's College Silver Medal | 2018 |
| University of Toronto Excellence Award | 2018 |
| St. Michael's College In-Course Scholarship | 2018 |
| Canadian Society for Chemistry Silver medal | 2018 |
| CQIQC Undergraduate Summer Reaserch Program | 2017 |
| University of Toronto Excellence Award | 2017 |
| F. E. Beamish Scholarship in Chemistry | 2017 |
| Buduchnist Credit Union Scholarship | 2017 |
| Ivan Szak Scholarship in Chemistry | 2017 |
| Michael Both Award for Outstanding Commitment to Dance | 2017 |
| John Melady Memorial Scholarship | 2017 |
| C. W. Burton In-Course Scholarship | 2017 |
| Gollop Memorial Undergraduate Scholarship in Chemistry | 2017 |
| Dean's List Scholar | 2017 |
| University of Toronto Excellence Award | 2016 |
| Kupcinet-Getz Research Scholarship | 2015 |
| University of Toronto Mississauga Honour Roll | 2015 |
| Erindale Admission Scholarship | 2014 |
| Scholarship of the President of Ukraine<br>*(awarded annually to approximately 250 highest achieving high school students out of over a million)* | 2014 |
| Lutsk's student of the year<br>*(awarded annually to the highest achieving high school graduate out of approximately 10,000)* | 2014 |
| First Prize at Intel-Eco Ukraine 2014, the national stage of Intel ISEF | 2014 |
| Gold medal at the International Ecology Project Olympiad | 2013 |

PUBLICATIONS

13. **Korol*, R.**; Chen, X.; Franco* I. High-frequency tails in spectral densities. *J. Phys. Chem. A* **2025**. DOI: 10.1021/acs.jpca.5c00943

12. Turner*, A.C.; **Korol, R.**; Bill, M.; Stolper, D.A. Stable isotope equilibria in dihydrogen-water-methane-ethane-propane system. Part 2: Experimental determination of hydrogen isotopic equilibrium for ethane-H2 from 30–200°C and propane-H2 from 75–200°C. *Geochim. et Cosmochim. Acta* **2025**, 396, 91-106. DOI: 10.1016/j.gca.2025.02.033

11. **Korol*, R.**; Turner, A.C.; Nandi, A.; Bowman, J.M.; Goddard III, W.A.; Stolper, D.A. Stable isotope equilibria in dihydrogen-water-methane-ethane-propane system. Part 1: Path-integral calculations with CCSD(T) quality potentials. *Geochim. et Cosmochim. Acta* **2025**, 396, 71-90. DOI: 10.1016/j.gca.2025.02.028

10. Turner, A.C.; **Korol, R.**; Elbridge, D. L.; Bill, M.; Miller III, T.F.; Stolper* D.A. Experimental and theoretical determinations of hydrogen isotopic equilibrium in the system CH4-H2-H2O from 3 to 200°C. *Geochim. et Cosmochim. Acta* **2021**, 314, 223-269. DOI: 10.1016/j.gca.2021.04.026

9. (Editors' Pick) **Korol, R.**; Rosa-Raíces J.L., Bou-Rabee, N.; Miller* III, T.F. Dimension-free path-integral molecular dynamics without preconditioning. *J. Chem. Phys.* **2020**, 152, 104102. DOI: 10.1063/1.5134810

8. Elbridge, D. L.; **Korol, R.**, Lloyd, M.K.; Turner, A.C.; Webb, M.A.; Miller III, T.F.; Stolper* D.A. Comparison of Experimental vs Theoretical Abundances of $^{13}CH_3D$ and $^{12}CH_2D_2$ for Isotopically Equilibrated Systems from 1 to 500 °C. *ACS Earth Space Chem.* **2019**, 3 (12), 2747-2764. DOI: 10.1021/acsearthspacechem.9b00244

7. (Editors' Choice) Elbridge, D. L.; **Korol, R.**, Lloyd, M.K.; Turner, A.C.; Webb, M.A.; Miller III, T.F.; Stolper* D.A. Comparison of Experimental vs Theoretical Abundances of $^{13}CH_3D$ and $^{12}CH_2D_2$ for Isotopically Equilibrated Systems from 1 to 500 °C. *ACS Earth Space Chem.* **2019**, 3 (12), 2747-2764. DOI: 10.1021/acsearthspacechem.9b00244

6. (Editors' Pick) **Korol, R.**; Bou-Rabee, N.; Miller* III, T.F. Cayley modification for strongly stable path-integral and ring-polymer molecular dynamics. *J. Chem. Phys.* **2019**, 151 (12), 124103. DOI: 10.1063/1.5120282

5. **Korol R.**; Segal* D. Machine Learning Prediction of DNA Charge Transport. *J. Phys. Chem. B*, **2019**, 123 (13), pp 2801 — 2811. DOI: 10.1021/acs.jpcb.8b12557

4. **Korol, R.**; Segal*, D. From exhaustive simulations to key principles in DNA nanoelectronics. *J. Phys. Chem. C* **2018** 122 (8), 4206-4216. DOI: 10.1021/acs.jpcc.7b12744

3. **Korol, R.**; Kilgour, M.; Segal*, D. ProbeZT: Simulation of transport coefficients of molecular electronic junctions under environmental effects using Büttiker's probes. *Comp. Phys. Comm.* **2018** 224, 396-404. DOI: 10.1016/j.cpc.2017.10.005

2. **Korol, R.**; Kilgour, M.; Segal*, D. Thermopower Of Molecular Junctions: Tunneling To Hopping Crossover In DNA. *J. Chem. Phys.* **2016**, 145 (22), 224702. DOI: 10.1063/1.4971167

1. Longobardi, L.E.; Zatsepin, P.; **Korol, R.**; Liu, L.; Grimme, S.; Stephan* D.W. Reactions Of Boron-Derived Radicals With Nucleophiles. *J. Am. Chem. Soc.* **2016**, 139 (1), pp 426—435. DOI: 10.1021/jacs.6b11190

## Presentations and Awards

American Conference on Theoretical Chemistry, Chapel Hill, North Carolina 2024
Poster: "Analog Simulation of Open Quantum Dynamics"

Gray-Hill lecture at the Occidental college, Los Angeles, California. 2023
Award talk: "A window to Earth's past with the help of theoretical chemistry"

Canadian Chemistry Conference and Exhibition, Calgary, Canada 2022
Contributed talk: "Accurate quantum statistics from improved path-integrals in imaginary time"

Molecular Science Mini-meeting, Montreal, Canada 2022
Poster: "Dimension-free ring-polymer molecular dynamics"

ACS Spring meeting, San Diego, California 2022
Poster: "Accurate quantum statistics from improved path-integrals in imaginary time"

Geological and Planetary Sciences seminar at Caltech, Pasadena, California 2022
Invited talk: "$D$ and $^{13}C$ exchange equilibria using Path-Integral Monte-Carlo"

Berkeley Statistical Mechanics Meeting 2020
Poster: "Cayley modification for strongly stable path-integral molecular dynamics"

CECAM BioMolecular Electronics Conference, Madrid, Spain 2018
Poster: "Principles of Charge Transport in DNA: from extensive simulations to neural networkds"

28$^{th}$ Canadian Symposium on Theoretical and Computational Chemistry, Windsor, Canada 2018
Poster prize: "Charge transport in DNA: From comprehensive simulations to key principles"

100$^{th}$ Canadian Chemistry Conference, Toronto, Canada 2017
Poster prize: "Tunneling to Hopping Crossover in Thermopower of DNA Molecular Junctions"

Chemical Biophysics Symposium, Toronto, Canada 2017
Contributed talk: "DNA Molecular Junctions: Tunneling to Hopping Crossover"

33$^{rd}$ Symposium on Chemical Physics, Waterloo, Canada 2017
Contributed talk: "Probing mechanisms of charge transport in DNA with Landauer-Büttiker formalism"

45th Southern Ontario Undergraduate Student Chemistry Conference, Toronto, Canada 2017
1$^{st}$ prize talk: "Tunneling to Hopping Crossover in DNA & DNA-like molecular junctions"

## Community Volunteer Initiatives

Spearheaded and coordinated humanitarian supplies shipment to Ukraine 2022–2023
from Caltech campus and beyond

Volunteer at the Nova Ukraine non-profit, Stanford, California 2021–2023
Website development, established and coordinated partnership with *Teach for Ukraine*

Volunteer at the Teach for Ukraine nonprofit, Kyiv, Ukraine 2021–2022
Recruited and interviewed candidate teachers at the remote interview stage

International student orientation leader 2019, 2020

"Big sibling" mentor for the incoming graduate students at Caltech 2019, 2020

Science outreach program volunteer through Caltech Y 2018–2020

High-school tutoring with CAUSE Tutoring non-profit 2018–2019

University of Toronto Peer Tutoring group tutor 2015–2018

## Service

Student Representative at the Chemistry Department Advisory Committee 2016–2017

2$^{nd}$ year representative at the Chemistry student union 2016–2017

Board member of the *Chemistry Connections* student group 2015–2016

## Teaching

*Course development:* Computational chemistry labs, Chem3 at Caltech 2022
Focus on structure-function relations and the dangers of approximations.

High School Teacher, Rotman Arts and Science School, Vaughan, Canada 2020–2022
Academic stream, grade 11 and 12 Chemistry, Grade 10 Science.
Student placed 3rd in Vaughan, top 200 in Canada at the Avogadro chemistry contest

International Chemistry Olympiad Coach
Canadian National Team (4 students) – 2 bronze, 1 silver medals Spring 2018
Ukrainian National team (1 student) – bronze medal Spring 2014

Private tutoring of Chemistry, Physics and Math 2014–2018
High school students: accepted to University college (UK), Columbia University (USA) and others

Chemical Biology summer school, Lutsk, Ukraine Summer 2015
Designed problems and experiments to help high school students master key concepts in chemistry

## Peer Review

Physical Review Letters
Physical Review A
Physical Review B (joint review)
Physical Review E
Chemical geology
Physical chemistry chemical physics
Rapid communications in mass spectrometry
ACS Physical Chemistry Au

## Summer Schools and Workshops

Condensed Phase Dynamics Workshop at TSRC (Virtual) 2020

Theoretical Chemistry School at TSRC, Telluride, Colorado 2019

Weizmann Institute of Science, Rehovot, Israel 2015
Kupcinet-Getz Scholar at Rubtchinski lab

## Employment

High School Teacher, Rotman Arts and Science School, Vaughan, Canada 2020–2022

Research Assistant, Department of Linguistics, University of Toronto 2016–2018
Heritage language variation and change project

## Extra curriculars

Rock clibmbing, weightlifting since 2014
Guitar, base since 2012
Ukrainian folk dance since 2004

## Languages

Fluent in Ukrainian, English & Russian

## Computer Languages

Python, C++, MATLAB, FORTRAN, Mathematica, Bash;
Web development (PHP & django, HTML, CSS, JS)