Roman Korol 🔗

✉ roman.korol@rochester.edu
📞 +1 626 219 3728

University of Rochester
Department of Chemistry
Hutchison Hall
Rochester, NY 14620

CURRENT POSITION	**University of Rochester**, Rochester, New York Postdoctoral Fellow, 2023-2025
FUTURE POSITION	**Université de Sherbrooke**, Sherbrooke, Quebec, Canada Assistant Professor, starting in January of 2026
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

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 *(awarded annually to approximately 250 highest achieving high school students out of over a million)*	2014
Lutsk's student of the year *(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

15. **Korol*, R.**; Nichol*, J..; Franco* I. Hybrid singlet-triplet qubits enable fault-tolerant single-pulse CNOT gate. *In review*

14. Tiwari, V.; **Korol, R.**; Franco* I. Robust purely optical signatures of Floquet-Bloch states in crystals. *In review*

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](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](10.1016/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](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](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](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](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](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 Poster: "Analog Simulation of Open Quantum Dynamics"	2024
	Gray-Hill lecture at the Occidental college, Los Angeles, California. <u>Award talk:</u> "A window to Earth's past with the help of theoretical chemistry"	2023
	Canadian Chemistry Conference and Exhibition, Calgary, Canada Contributed talk: "Accurate quantum statistics from improved path-integrals in imaginary time"	2022
	Molecular Science Mini-meeting, Montreal, Canada Poster: "Dimension-free ring-polymer molecular dynamics"	2022
	ACS Spring meeting, San Diego, California Poster: "Accurate quantum statistics from improved path-integrals in imaginary time"	2022
	Geological and Planetary Sciences seminar at Caltech, Pasadena, California <u>Invited talk:</u> "D and ^{13}C exchange equilibria using Path-Integral Monte-Carlo"	2022
	Berkeley Statistical Mechanics Meeting Poster: "Cayley modification for strongly stable path-integral molecular dynamics"	2020
	CECAM BioMolecular Electronics Conference, Madrid, Spain Poster: "Principles of Charge Transport in DNA: from extensive simulations to neural networkds"	2018
	28th Canadian Symposium on Theoretical and Computational Chemistry, Windsor, Canada <u>Poster prize:</u> "Charge transport in DNA: From comprehensive simulations to key principles"	2018
	100th Canadian Chemistry Conference, Toronto, Canada <u>Poster prize:</u> "Tunneling to Hopping Crossover in Thermopower of DNA Molecular Junctions"	2017
	Chemical Biophysics Symposium, Toronto, Canada Contributed talk: "DNA Molecular Junctions: Tunneling to Hopping Crossover"	2017
	33rd Symposium on Chemical Physics, Waterloo, Canada Contributed talk: "Probing mechanisms of charge transport in DNA with Landauer-Büttiker formalism"	2017
	45th Southern Ontario Undergraduate Student Chemistry Conference, Toronto, Canada <u>1st prize talk:</u> "Tunneling to Hopping Crossover in DNA & DNA-like molecular junctions"	2017
COMMUNITY VOLUNTEER INITIATIVES	Spearheaded and coordinated humanitarian supplies shipment to Ukraine 🔗 from Caltech campus and beyond	2022–2023
	Volunteer at the Nova Ukraine non-profit, Stanford, California Website development, established and coordinated partnership with *Teach for Ukraine*	2021–2023
	Volunteer at the Teach for Ukraine nonprofit, Kyiv, Ukraine Recruited and interviewed candidate teachers at the remote interview stage	2021–2022
	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
	2nd 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

ACS journals: ACS Physical Chemistry Au
APS journals: Physical Review Letters, Physical Review A, B, and E
Elsevier journals: Organic Geochemistry, Chemical Geology
RSC journals: Physical chemistry chemical physics
Wiley journals: Rapid communications in mass spectrometry

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)