

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

PUBLICATIONS

13. **Korol, R.**; Chen, X.; Franco I. High-frequency tails in spectral densities. *In review*. ArXiv: [arXiv:2405.01381](https://arxiv.org/abs/2405.01381)
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. *In review*.
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. *In review*.
10. **Korol, R.V.**; Yanchuk O.M; Marchuk O.V. Orlov V.F; Moroz I.A. and Vyshnevskiy O.A. Size Stabilizers in Two-electrode Synthesis of ZnO Nanorods. *Phys. & Chem. of Solid State* **2021**, 22(2), pp 380–387. DOI: [10.15330/pcss.22.2.380-387](https://doi.org/10.15330/pcss.22.2.380-387)
9. 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**. DOI: [10.1016/j.gca.2021.04.026](https://doi.org/10.1016/j.gca.2021.04.026)
8. (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](https://doi.org/10.1063/1.5134810)
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 ¹³CH₃D and ¹²CH₂D₂ for Isotopically Equilibrated Systems from 1 to 500 °C. *ACS Earth Space Chem.* **2019**, 3 (12), 2747–2764. DOI: [10.1021/acsearthspacechem.9b00244](https://doi.org/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](https://doi.org/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.jpcc.8b12557](https://doi.org/10.1021/acs.jpcc.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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1021/jacs.6b11190)

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 Research 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
	Kupcinet-Getz Research Scholarship	2015
	University of Toronto Mississauga Honour Roll	2015
	Erindale Admission Scholarship	2014
	Scholarship of the President of Ukraine <i>(awarded annually to approximately 250 highest achieving high school students out of over a million)</i>	2014
	Lutsk's student of the year <i>(awarded annually to the highest achieving high school graduate out of approximately 10,000)</i>	2014
	First Prize at Intel-Eco Ukraine 2014, the national stage of Intel ISEF	2014
	Gold medal at the International Ecology Project Olympiad	2013
TEACHING	<i>Course development:</i> Computational chemistry labs, Chem3 at Caltech Focus on structure-function relations and the dangers of approximations.	2022
	High School Teacher, Rotman Arts and Science School, Vaughan, Canada Academic stream, grade 11 and 12 Chemistry, Grade 10 Science. Student placed 3rd in Vaughan, top 200 in Canada at the Avogadro chemistry contest	2020–2022
	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 High school students: accepted to University college (UK), Columbia University (USA) and others	2014–2018
	Chemical Biology summer school, Lutsk, Ukraine Designed problems and experiments to help high school students master key concepts in chemistry	Summer 2015

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
	<u>Award talk</u> : "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
	<u>Invited talk</u> : " 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 networks"	
	28 th Canadian Symposium on Theoretical and Computational Chemistry, Windsor, Canada	2018
	<u>Poster prize</u> : "Charge transport in DNA: From comprehensive simulations to key principles"	
	100 th Canadian Chemistry Conference , Toronto, Canada	2017
	<u>Poster prize</u> : "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"	
	45 th Southern Ontario Undergraduate Student Chemistry Conference , Toronto, Canada	2017
	<u>1st prize talk</u> : "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 <i>Teach for Ukraine</i>	
	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
SERVICE	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
	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 <i>Chemistry Connections</i> student group	2015–2016

PEER REVIEW	Physical Review B (joint review) 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) Theoretical Chemistry School at TSRC , Telluride, Colorado Weizmann Institute of Science, Rehovot, Israel Kupcinet-Getz Scholar at Rubtchinski lab	2020 2019 2015
EMPLOYMENT	High School Teacher, Rotman Arts and Science School, Vaughan, Canada Research Assistant, Department of Linguistics, University of Toronto Heritage language variation and change project	2020–2022 2016–2018
EXTRA CURRICULARS	Rock climbing, weightlifting Guitar, base Ukrainian folk dance	since 2014 since 2012 since 2004
LANGUAGES	Fluent in Ukrainian, English & Russian	
COMPUTER LANGUAGES	Python, C++, MATLAB, FORTRAN, Mathematica, Bash; Web development (PHP & django, HTML, CSS, JS)	