Research Summary

Chemical Physics Theory Group, University of Toronto Fall 2017 – Spring 2018
Senior thesis project under the supervision of Professor Jeremy Schofield

Topic: Using Fokker-Plank dynamics to model protein folding
Work done so far: Validated the model using exact solution of the Focker-Planck equation for the simple potentials. Moving towards studying sharp, but continuous potentials.

Chemical Physics Theory Group, University of Toronto Summer 2016 – Fall 2017
Two summer projects, funded by Excellence Research Fund (both) and Center for Quantum Information and Quantum Control (the second one) under the supervision of Professor Dvira Segal

Work done:

1. Going beyond Landauer (scattering) formalism with the help of Butticker probes to describe charge transport in the intermediate quantum-classical regime. System studied: single molecule DNA junctions under thermoelectric bias.
2. Continuing investigation of the junctions based on the DNA and other polymers; preparation of our quantum transport code for the publication; spin filtering using the chirality of the DNA helix; pushing the limits of minimum models for quantum refrigerator: investigation of a two-level system with three reservoirs under the strong system-bath coupling.

Publications and Presentations:

- **Korol R.**; Segal D. Machine Learning Prediction of DNA Charge Transport. *J. Phys. Chem. B*, **2019**, 123 (13), pp 2801 — 2811. 10.1021/acs.jpcb.8b12557
  - Poster at the Berkeley Mini Stat Mech Meeting (2018)
- **Korol, R.**; Kilgour, M.; Segal, D. Thermopower Of Molecular Junctions: Tunneling To Hopping Crossover In DNA. *J. Chem. Phys* 145, 224702 **2016**. 10.1063/1.4971167
  - Contributed talk at 45th Southern Ontario Undergraduate Student Chemistry Conference (York University)
  - Contributed talk at Chemical Biophysics Symposium–2017 (University of Toronto)
  - Poster at the 100th Canadian Chemistry Conference (Toronto)
- **Korol, R.**; Kilgour, M.; Segal, D. ProbeZT: Simulation of transport coefficients of molecular electronic junctions under environmental effects using Buttiker's probes. *Comp. Phys. Comm.* (in press) **2017** 10.1016/j.cpc.2017.10.005
- **Korol R.**; Segal D. Electrical conduction through DNA molecules: An exhaustive computational study (manuscript in preparation)
  - Contributed talk at 33rd Symposium on Chemical Physics, U of Waterloo

Inorganic Synthetic Laboratory, University of Toronto *Winter – Spring 2016*
Volunteering under direct supervision of Dr. Lauren Longobardi, PI: Professor Doug Stephan

Work done: Synthesis of radicals containing Boron (in the glove due to water and air-sensitivity of the reagents and products), running the reaction scopes, NMR analysis, various separations.

Publication:

- 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. 10.1021/jacs.6b11190

Organic Materials Laboratory, Weizmann Institute of Science, Rehovot, Israel *Summer 2015*
Kupcinet-Getz Summer School under the supervision of Professor Boris Rybtchinski
Topic: self-assembly of organic nanocrystals, their fluorescence and non-linear optics

Work done: Synthesis and purification of the perylene diimide (PDI) dye with a non-centrosymmetric lattice, UV-VIS and fluorescence spectroscopy studying its optical properties in various solvents; SEM and TEM imaging of the self-assemblies (under the supervision of Shacked Rosenne and Dr. Haim Weissman)

Inorganic Synthetic Laboratory, University of Toronto Mississauga *Fall 2014 – Spring 2015*
Volunteering under the supervision of David Armstrong, PI: Associate Professor Ulrich Fekl
Topic: Functionalization of halogenated adamantanes

Work done: Synthesis of mono- and dibromoadamantane, reacting these with the alkyl metal nucleophiles.

Inorganic materials Laboratory, Eastern European National University, Lutsk, Ukraine
Summer 2013 – Spring 2014
A project in the Junior Academy of Sciences of Ukraine under the supervision of Dr. Oleksandr Yanchuk

Work done: Synthesis of nanoparticles of ZnO using a two-electrode electrolytic cell set-up under various conditions. *Publications and presentations:*

- **Korol, R.**; Marchuk, V.; Urubkov I.V.; Yanchuk O.M. Controlling the Size and Morphology of ZnO Nanorods in Two-electrode Synthesis Using Auxiliary Stabilizers (manuscript in preparation)
  - Poster at the National Ecology Olympiad, Vinnytsa, Ukraine
  - Poster at the Intel-Eco Ukraine - the national stage of the international Intel ISEF, Kiev, Ukraine
  - Contributed talk at the National competition, organized by the Junior Academy of Sciences of Ukraine

Biological Chemistry Laboratory, Eastern European National University, Lutsk, Ukraine
Summer 2012 – Spring 2013
A project in the Junior Academy of Sciences of Ukraine under the supervision of Dr. Vasyl Voytiuk and Dr. Halyna Yagenska

Topic: Plant Leaves Morphology and Biochemistry in the Urban Atmosphere

Work done: sample gathering and preparation (fieldwork), extraction of pigments, UV-VIS spectroscopic analysis (labwork)

Publications and presentations:

- **Korol, R.**; Repetylo, I.; Yagenska H. Plant Leaves Morphology and Biochemistry in the Urban Atmosphere. 21st International Environmental Project Olympiad project book, 2013, Istanbul, Turkey
  - Poster at the INEPO-2013, Instanbul, Turkey