

CURRICULUM VITAE

A. BIOGRAPHICAL INFORMATION

1. PERSONAL

Name: Dvira Segal
University Address: Department of Chemistry, University of Toronto,
80 St. George Street, Toronto, Ontario, M5S 3H6
Office Phone: 416 946 0559
Email address: dsegal@chem.utoronto.ca

2. DEGREES

2004 Ph.D. (direct program) in Chemistry, Tel Aviv University
Title of Graduate thesis: Electron transfer in molecular conductors
Supervisor: Professor Abraham Nitzan

1998 B.Sc. in Chemistry Major-Computer Science Minor,
CUM LAUDE, Tel Aviv University

3. EMPLOYMENT

July 2012- Associate Professor, Department of Chemistry, University of Toronto
July 2007-2012 Assistant Professor, Department of Chemistry, University of Toronto
2006-2007 Postdoctoral Fellow
Department of Chemistry, Columbia University, New York
2003-2005 Concurrent Postdoc position in:
Chemical Physics Department, Weizmann Institute of Science, Rehovot, Israel
Department of Chemistry University of British Columbia, Vancouver, Canada

4. HONOURS

2014-2019 Canada Research Chair (Tier II) in Theoretical Chemistry
2010-2012 Alfred P. Sloan Research Fellow
2010-2015 Early Research Award
2000-2003 The Clore scholarship for Ph.D. students
1995, 1996 The Dean's list for academic achievements in the
Faculty of Exact Sciences, Tel-Aviv University

5. PROFESSIONAL AFFILIATIONS AND ACTIVITIES

Chemical Institute of Canada: Member

B. ACADEMIC HISTORY

6A. RESEARCH ENDEAVOURS

Field: Theoretical Chemical Physics

(a) **Quantum transport and dissipation.** Our research is focused on the development of analytical and computational methods for describing charge and energy transfer in condensed phases. This includes: (i) Formulation of general methodologies, for following the dynamics of many-body quantum systems driven out-of-equilibrium by a potential bias or/and a temperature gradient. (ii) Analysis of simple model systems, for elucidating basic transport and dissipation mechanisms. This work is linked to the field of “molecular electronics”. Practically, we study mechanisms of single-molecule conduction, explore molecular thermoelectrics, and provide physical information from noise measurements.

(b) **Energy transfer at the nanoscale.** We aim to understand the relationship between a microscopic description of a system and its energy transport characteristics, in the quantum regime, going beyond the particular realization. This includes the study of phononic, excitonic, and photonic energy flow in low dimensional systems. We are interested in elucidating nonlinear energy transport effects such as thermal rectification effect, and in modeling molecular machinery, pumps and engines. Our work connects with the fields of “quantum thermodynamics” and “nanophonics”.

(c) **Quantum statistical mechanics.** We are interested in validating the heat exchange fluctuation theorems, quantifying second law violation, in strongly-coupled many-body quantum systems. With the acquired cumulant generating function we calculate the heat current and its moments.

(d) **Finite time thermodynamics.** We explore fundamental issues in classical and quantum thermodynamics such as the universality of the maximum-power efficiency, Landauer’s erasure principle, and information theory exorcism of Maxwell’s demon.

6B. RESEARCH AWARDS: CURRENT

Agency, Type and Title	Beginning date	End Date	Total	PI
Natural Sciences and Engineering Research Council Canada: Discovery Grant Energy harvesting at the nanoscale:: From principles to functions	April 2016	April 2020	\$ 230,000	Segal
Natural Science and Engineering Research Council Canada Canada Research Chair (Tier II) Theoretical Chemistry	April 2014	April 2019	\$ 500,000	Segal
University of Toronto Start-up Funds	July 2007	Open	\$ 200,000	Segal

C. SCHOLARLY AND PROFESSIONAL WORK

Names of students trained by D. Segal are underlined>.

7. REFEREED PUBLICATIONS

A. Articles

1. M. Galperin, D. Segal, and A. Nitzan,
Perturbation theory approach to tunneling: Direct and resonance transmission in super-exchange models,
J. Chem. Phys. **111**, 1569-1579 (1999).
2. D. Segal, A. Nitzan, W. B. Davis, M. R. Wasielewsky, and M. A. Ratner,
Electron transfer rates in bridged molecular systems: A steady state analysis of coherent tunneling and thermal transitions,
J. Phys. Chem. B. **104**, 3817-3829 (2000).
3. D. Segal, A. Nitzan, M. Ratner, and W. B. Davis,
Activated conduction in microscopic molecular junctions,
J. Phys. Chem. B. **104**, 2790-2793 (2000).
4. D. Segal and A. Nitzan,
Steady state quantum mechanics of thermally relaxing systems,
Chem. Phys. **268**, 315-335 (2001).
5. D. Segal and A. Nitzan,
Conduction in molecular junctions: Inelastic effects,
Chem. Phys. **281**, 235-256 (2002).
6. D. Segal and A. Nitzan,
Heating in current carrying molecular junctions,
J. Chem. Phys. **117**, 3915-3927 (2002).
7. D. Segal, A. Nitzan, and P. Hänggi,
Thermal conductance through molecular wires,
J. Chem. Phys. **119**, 6840-6855 (2003).
8. D. Segal, P. Král, and M. Shapiro,
Shaping of detached image states above nanowires,
Phys. Rev. B **69**, 153405-0 - 153405-4 (2004).
9. D. Segal, P. Král, and M. Shapiro,
Electric and magnetic-field tuning of tubular image states around suspended nanowires,
Chem. Phys. Lett. **392**, 314-318 (2004).
10. D. Segal, B. E. Granger, H. Sadeghpour, P. Král, and M. Shapiro,
Tunable bands of electronic image states in nanowire lattices,
Phys. Rev. Lett. **94**, 016402-1 - 016402-4 (2005).
11. D. Segal and A. Nitzan,
Spin-boson thermal rectifier,
Phys. Rev. Lett. **94**, 034301-1 - 034301-4 (2005).
12. D. Segal and A. Nitzan,
Heat rectification in molecular junctions,
J. Chem. Phys. **122**, 194704-1 - 194704-12 (2005).

13. D. Segal, P. Král, and M. Shapiro,
Ultraslow relaxation of angular momenta in tubular image states,
Surf. Sci. **577**, 86-92 (2005).
14. D. Segal, P. Král, and M. Shapiro,
Reentrant onset of chaos in tubular image states,
J. Chem. Phys. **122**, 134705-1 - 134705-6 (2005).
15. D. Segal,
Thermoelectric effect in molecular junctions: A tool for revealing transport mechanisms,
Phys. Rev. B **72**, 165426-1 - 165426-7 (2005).
16. D. Segal and A. Nitzan,
Molecular heat pump,
Phys. Rev. E **73**, 026109-1 - 026109-9 (2006).
17. D. Segal and M. Shapiro,
Trapping of a single electron in a nanoscale Paul trap,
Nano Lett. **6**, 1622-1626 (2006).
18. D. Segal, T. Seideman, G. Kurizki, and M. Shapiro,
Enhancement of nuclear tunneling through Coulomb-barriers using molecular-cages,
Chem. Phys. Lett. **420**, 241-244 (2006).
19. D. Segal,
Heat flow in nonlinear molecular junctions: Master equation analysis,
Phys. Rev. B **73**, 205415-1 - 205415-9 (2006).
20. D. Segal, P. Král, and M. Shapiro,
Electric control on the nanoscale using tubular image states,
Israel Journal of Chemistry **47**, 105-110 (2007). (cover)
21. D. Segal and D. R. Reichman,
Zeno and anti-Zeno effects in spin-bath models,
Phys. Rev. A **76**, 012109-1 - 012109-6 (2007).
22. D. Segal, A. J. Millis, and D. R. Reichman,
Non-equilibrium quantum dissipation in spin-fermion systems,
Phys. Rev. B **76**, 195316-1 - 195316-21 (2007).
23. D. Segal,
Nonlinear thermal control in an N -terminal junction,
Phys. Rev. E **77**, 021103-1 - 021103-6 (2008).
24. D. Segal,
Single mode heat rectifier: Controlling energy flow between electronic conductors,
Phys. Rev. Lett. **100**, 105901-1 - 105901-4 (2008).
25. D. Segal,
Thermal conduction in molecular chains: Non-Markovian effects,
J. Chem. Phys. **128**, 224710-1 - 224710-8 (2008).
26. L.-A. Wu and D. Segal,
Fourier's law of heat conduction: Quantum mechanical master equation analysis,
Phys. Rev. E **77**, 060101(R)-1 - 060101(R)-4 (2008).
27. D. Segal,
Stochastic pumping of heat: Approaching the Carnot efficiency,
Phys. Rev. Lett. **101**, 260601-1 - 260601-4 (2008).

28. L.-A. Wu and D. Segal,
Energy flux operator: Current conservation and the formal Fourier's law,
J. Phys. A: Math. Theor. **42**, 025302 (2009). (15 pages)
29. D. Segal,
Absence of thermal rectification in asymmetric harmonic chains with self consistent reservoirs,
Phys. Rev. E **79**, 012103-1 - 012103-4 (2009).
30. L.-A. Wu and D. Segal,
Sufficient conditions for thermal rectification in hybrid quantum structures,
Phys. Rev. Lett. **102**, 095503-1 - 095503-4 (2009).
31. L.-A. Wu, S. S. Wu, and D. Segal,
Looking into DNA breathing dynamics via quantum physics,
Phys. Rev. E **79**, 061901-1 - 061901-5 (2009).
32. D. Segal,
Vibrational relaxation in the Kubo oscillator: Stochastic pumping of heat,
J. Chem. Phys. **130**, 134510-1 - 134510-10 (2009).
33. L.-A. Wu, C. X. Yu, and D. Segal,
Nonlinear quantum heat transfer in hybrid structures: Sufficient conditions for thermal rectification,
Phys. Rev. E **80**, 041103-1 - 041103-12 (2009).
34. C. X. Yu, L.-A. Wu, and D. Segal,
Symmetry properties of the heat current in non-ballistic asymmetric junctions: A case study,
Physics Letters A **374**, 765-769 (2010).
35. L. Nicolin and D. Segal,
Thermal conductance of the Fermi-Pasta-Ulam chains: Atomic to mesoscopic transition,
Phys. Rev. E (Rapid Comm.) **81**, 040102-1- 040102-4 (2010).
36. L.-A. Wu, D. Segal, Inigo L. Egusquiza, and P. Brumer,
Universality in exact quantum state population dynamics and control,
Phys. Rev. A **82**, 032307 (2010).
37. Y. Zhou and D. Segal,
Minimal model of a heat engine: An information theory approach,
Phys. Rev. E **82**, 011120-1 - 011120-5 (2010).
38. Y. Zhou and D. Segal,
Interface effects in thermal conduction through molecular junctions: Numerical simulations,
J. Chem. Phys. **133**, 094101-1 - 094101-9 (2010).
39. D. Segal, A. J. Millis, and D. R. Reichman,
Numerically exact path integral simulation of non equilibrium quantum transport and dissipation,
Phys. Rev. B **82**, 205323-1 - 205323-13 (2010).
Editors' Suggestion
40. L.-A. Wu and D. Segal,
Quantum heat transfer: A Born-Oppenheimer method,
Phys. Rev. E **83**, 051114-1 - 051114-5 (2011).
41. M. Bandyopadhyay, S. Gupta and D. Segal,
DNA breathing dynamics: Analytic results for distribution functions of relevant Brownian functionals,
Phys. Rev. E **83**, 0313905-1 - 0313905-12 (2011).
42. D. Segal, A. J. Millis, and D. R. Reichman,
Nonequilibrium transport in quantum impurity models: exact path integral simulations,
Phys. Chem. Chem. Phys. **13**, 14378-14386 (2011). (Themed Issue on "Molecular Electronics")

43. L.-A. Wu and D. Segal,
Quantum effects in thermal conduction: Nonequilibrium quantum discord and entanglement,
Phys. Rev. A **84**, 012319-1 - 012319-6 (2011).
44. M. Bandyopadhyay and D. Segal,
Quantum heat transfer in harmonic chains with self consistent reservoirs: Exact numerical simulations,
Phys. Rev. E **84**, 011151-1 - 011151-8 (2011).
45. L. Nicolin and D. Segal,
Non-equilibrium spin-boson model: counting statistics and the heat exchange fluctuation theorem,
J. Chem. Phys. **135**, 164106-1 - 164106-14 (2011).
46. L. Nicolin and D. Segal,
Quantum fluctuation theorem for heat exchange in the strong coupling regime,
Phys. Rev. B **84**, 161414-1 - 161414-4 (2011).
47. C. X. Yu, L.-A. Wu, and D. Segal,
Theory of energy transfer in spin chains: From superexchange to ballistic motion
J. Chem. Phys., **135**, 234508-1 - 234508-13 (2011).
48. S. Bedkihal and D. Segal,
Dynamics of coherences in the interacting double-dot Aharonov-Bohm interferometer: Exact numerical simulations
Phys. Rev. B **85**, 155324-1 - 155324-10 (2012).
49. S. Garmon, I. Rotter, N. Hatano, and D. Segal,
Analysis technique for exceptional points in open quantum systems and QPT analogy for the appearance of irreversibility
Int. J. of Theo. Phys. **51** 3536 - 3550 (2012).
50. L. Simine and D. Segal,
Vibrational cooling, heating, and instability in molecular conducting junctions: Full counting statistics analysis
Phys. Chem. Chem. Phys. **14** , 13820 - 13834 (2012).
51. M. Kulkarni, K. L. Tiwari, and D. Segal,
Towards equilibration and thermalization between finite quantum systems: The role of dephasing effects and inelastic interactions,
Phys. Rev. B **86**, 155424 (2012).
52. S. Garmon, T. Petrosky, L. Simine, and D. Segal,
Amplification of non-Markovian decay due to bound state absorption into continuum,
Fortschritte der Physik - Progress of Physics **61**, 261275 (2013).
53. M. Kulkarni, K. L. Tiwari, and D. Segal,
Full density matrix dynamics for large quantum systems: Interactions, Decoherence and Inelastic effects,
New J. Phys. **15** 013014 (2013).
54. L.-A. Wu, C. X. Yu, and D. Segal,
Exact dynamics of interacting qubits in a thermal environment: Results beyond the weak coupling limit,
New J. Phys. **15** 023044 (2013).
55. L.-A. Wu, D. Segal, and P. Brumer,
Ground state cooling is not possible given initial system-thermal bath factorization,
Scientific Reports **3**, 1824 (2013). (3 pages)

56. S. Bedkihal, M. Bandyopadhyay, and D. Segal,
Flux-dependent occupations and occupation difference in geometrically symmetric and energy de-
generate double-dot Aharonov-Bohm interferometers,
Phys. Rev. B **87**, 045418-1 - 045418-12 (2013).
57. D. Segal,
Qubit-mediated energy transfer between thermal reservoirs: beyond Markovian Master equation,
Phys. Rev. B **87**, 195436-1 - 195436-8 (2013).
58. L. Simine and D. Segal,
Path-integral simulations with fermionic and bosonic reservoirs: Transport and dissipation in molec-
ular electronic junctions,
J. Chem. Phys. **138**, 214111 (2013). (17 pages)
59. S. Bedkihal, M. Bandyopadhyay, and D. Segal,
Magnetic field symmetries of nonlinear transport with elastic and inelastic scattering,
Phys. Rev. B **88**, 155407-1:155407-5 (2013).
60. S. Bedkihal, M. Bandyopadhyay, and D. Segal,
The probe technique far-from-equilibrium: Magnetic field symmetries of nonlinear transport,
The European Physical Journal B **86** 506 (2013). (18 pages)
61. A. Dodin, S. Garmon, L. Simine, and D. Segal,
Landau-Zener transitions mediated by an environment: population transfer and energy dissipation,
J. Chem. Phys. **140**, 124709 (2014). (10 pages)
62. D. Segal,
Two-level system in spin baths: Non-adiabatic dynamics and heat transport,
J. Chem. Phys. **140**, 164110 (2014). (12 pages)
63. L. Simine and D. Segal,
Electron transport in nanoscale junctions with local anharmonic modes,
J. Chem. Phys. **141**, 014704 (2014). (14 pages)
64. D. Segal,
Heat transfer in the spin-boson model: A comparative study in the incoherent tunneling regime,
Phys. Rev. E **90**, 012148 (2014). (6 pages)
65. N. Boudjada and D. Segal,
From dissipative dynamics to studies of heat transfer at the nanoscale,
J. Phys. Chem. A, **118** (47), 11323-11336 (2014).
66. S. Bedkihal and D. Segal,
Magnetotransport in Aharonov Bohm interferometers: Exact numerical simulations,
Phys. Rev. B **90**, 235411 (2014). (11 pages)
67. L. Simine, W. J. Chen, and D. Segal,
Can Seebeck coefficient identify quantum interference in molecular conduction?
J. Phys. Chem. C **119**, 12097-12108 (2015). (12 pages)
68. E. Taylor and D. Segal,
Quantum bounds on heat transport through nanojunctions,
Phys. Rev. Lett. **114**, 220401 (2015). (5 pages +SI)
69. J.-H. Jiang, B. K. Agarwalla, and D. Segal,
Efficiency statistics and bounds for systems with broken time-reversal symmetry,
Phys. Rev. Lett. **115**, 040601 (2015). (5 pages + SI)
70. M. Kilgour and D. Segal,
Charge transport in molecular junctions: From tunneling to hopping with the probe technique,
J. Chem. Phys. **143**, 024111 (2015). (16 pages)

71. J.-H. Jiang, M. Kulkarni, D. Segal, and J. Imry,
Phonon-thermoelectric transistors and rectifiers,
Phys. Rev. B **92**, 045309 (2015). (9 pages)
72. E. Taylor and D. Segal,
Thermoelectric performance of strongly-correlated quantum impurity models,
Phys. Rev. B **92**, 125401 (2015). (10 pages)
73. J. Jing, D. Segal, B. Li, and L.-A. Wu,
Transient unidirectional energy flow and diode-like phenomenon induced by non-Markovian environments,
Scientific Reports **5**, 15332 (2015). (8 pages)
74. B. K. Agarwalla, J.-H. Jiang, and D. Segal,
Thermoelectricity in molecular junctions with harmonic and anharmonic modes,
Beilstein J. Nanotechnol. **6**, 2129-2139 (2015). (Thematic series on molecular machines and devices).
75. M. Kilgour and D. Segal,
Tunneling diodes with environmental effects,
J. Phys. Chem. C **119**, 25291-25297 (2015). (7 pages)
76. B. K. Agarwalla, J.-H. Jiang and D. Segal,
Full counting statistics of vibrationally-assisted electronic conduction: transport and fluctuations of the thermoelectric efficiency,
Phys. Rev. B **92**, 245418 (2015). (18 pages)
77. B. K. Agarwalla and D. Segal,
Reconciling perturbative approaches in phonon-assisted transport junctions,
J. Chem. Phys. **144**, 074102 (2016). (13 pages)
78. D. Segal and B. K. Agarwalla,
Vibrational heat transport in molecular junctions,
Annu. Rev. Phys. Chem. **67**, 185-209 (2016). (25 pages)
79. M. Kilgour and D. Segal,
Inelastic effects in molecular transport junctions: The probe technique at high bias,
J. Chem. Phys. **144**, 124107 (2016). (11 pages)
80. B. K. Agarwalla, M. Kulkarni, S. Mukamel, and D. Segal,
Tunable photonic cavity coupled to a voltage-biased double quantum dot system: Diagrammatic NEGF approach,
Phys. Rev. B **94**, 035434 (2016). (13 pages)
81. B. K. Agarwalla, M. Kulkarni, S. Mukamel, and D. Segal,
Giant photon gain in large-scale quantum dot circuit-QED systems,
Phys. Rev. B **94**, 121305(R) (2016) (4 pages).
82. H. Kim, M. Kilgour, and D. Segal,
Intermediate coherent-incoherent charge transport: DNA as a case study,
J. Phys. Chem. C **120** (42), 23951-23962 (2016).
83. R. Korol, M. Kilgour, and D. Segal,
Thermopower of molecular junctions: Tunneling to hopping crossover in DNA,
J. Chem. Phys. **145**, 224702 (2016). (12 pages)
84. H. Friedman, B. K. Agarwalla, D. Segal,
Effects of vibrational anharmonicity on molecular electronic conduction and thermoelectric efficiency,
J. Chem. Phys. **146**, 092303 (2017). (17 pages)

85. B. K. Agarwalla and D. Segal,
Energy current and its statistics in the nonequilibrium spin-boson model: Majorana fermion representation,
New J. Phys., in press. (2017) (14 pages). arXiv:1612.01008
86. H. Kim and D. Segal,
Controlling charge transport mechanisms in molecular junctions: Distilling thermally-induced hopping from coherent-resonant conduction,
J. Chem. Phys. **146**, 164702 (2017).

SI=supporting information

8. NON-REFEREED PUBLICATIONS

A. Articles

1. Inelastic effects in molecular conductors,
D. Segal and A. Nitzan,
Single Molecule **3**, 321 (2002).
2. P. Král, D. Segal, M. Shapiro, I. Thanopoulos, B. E. Granger, and H. R. Sadeghpour,
Bands of image states in nanowire lattices and infrared-control of proteins on nanotube ropes, Fullerenes, nanotubes, and carbon nanostructures **13**, 267-274 (2005).
3. A tribute to Paul Brumer in the Canadian Journal of Chemistry, D. Segal (Guest Editor), Can. J. Chem, **92**(2) (2014).
4. D. Segal,
Probing the limits of heat flow,
Science **355**, 1125-1126 (2017) (perspective).

B. Books Chapters

5. Tubular Image States and Trapping on the nanoscale,
D. Segal, P. Král, and M. Shapiro,
in "Coherent Control of Molecules" (2006), Collaborative Computational Project on Molecular Quantum Dynamics (CCP6), Daresbury, pp. 77-85, B. Lasorne and G.A. Worth, editors.
6. Theory, Experiment and Applications of Tubular Image States,
D. Segal, P. Král, and M. Shapiro,
"The Oxford Handbook of Nanoscience and Technology: Frontiers and Advances" A. V. Narlikar and Y. Y. Fu, editors. (Oxford University Press, Oxford, 2008)- Vol I, chap. 22, 823-864.
7. Heat transfer in nanostructures,
D. Segal,
"Proteins: Energy, heat and signal flow", (2009), D. Leitner and J. Straub, editors. CRC Press.

9. MANUSCRIPTS SUBMITTED

1. B. K. Agarwalla and D. Segal,
The Anderson impurity model out-of-equilibrium: Assessing the accuracy of simulation techniques with an exact current-occupation relation
arXiv:1704.00121

10. PAPERS PRESENTED at MEETINGS and SYMPOSIA (Invited) (2008-onward)

I receive invitations to present my work (invited speaker) in ~ 6 focused conferences, per year. I accept invitations and present my work in 2-3 meetings/year.

- National University of Singapore, Singapore, “Transmission of Information and Energy in Nonlinear and Complex Systems (TIENCS)” (May 2008)
Title of talk: “Single mode thermal rectifier: Energy exchange between metals”
- Helsinki University of Technology, Finland, Conference on “Micro and Nanocryogenics” (Aug. 2008)
Title of talk: “Single mode thermal rectifier: Energy exchange between metals”
- The 92nd Canadian Chemistry Conference and Exhibition, Hamilton, Ontario, Canada “Quantum Chemical Dynamics Symposium” (June 2009)
Title of talk: “Iterative path integral simulations of non-equilibrium transport and dissipation”
- Telluride, Colorado, Workshop on “Quantum Transport in Nanoscale Molecular System” (July 2009)
Title of talk: “Iterative path integral simulations of non-equilibrium transport and dissipation”
- UCSD, La Jolla, California, A meeting on “Optimization at a small scale” (July 2009)
Title of talk: “Energy transfer at the nanoscale: diodes and pumps”
- Stuttgart, Germany, International symposium “Quantum Thermodynamics: Energy and Information Flow at the Nano-Scale” (Sep. 2010)
Title of talk: “Minimal model of a heat engine: An information theory approach”
- Erice, Sicily, Italy, “New trends in nonlinear dynamics: Heat control and thermo-electric efficiency” HEAT2010 (Oct. 2010)
Title of talk: “Heat engines and thermal conductors: An information theory model”
- Snogeholm, Sweden, “Thermodynamics: Can macro learn from nano?” (May 2011)
Title of talk: “Quantum heat conduction in nonlinear systems: Steady state fluctuation theorem for the spin-boson model, and beyond”
- Telluride, Colorado, Workshop on “Chemistry and Dynamics in Complex Environments” (June 2011)
Title of talk: “Iterative path integral simulations of non-equilibrium transport and dissipation”
- Telluride, Colorado, Workshop on “Quantum Transport in Nanoscale Molecular Systems” (Aug. 2011)
Title of talk: “Off-resonance energy transfer in bridged junctions: Method and applications”
- Hebrew University, Israel Institute for Advanced Studies, Jerusalem, Workshop on Molecular Electronics (July 2012)
Title of talk: “Approaching thermal equilibrium between finite quantum systems: The role of dephasing effects and inelastic interactions”
- Telluride, Colorado, Workshop on “Quantum Transport in Nanoscale Molecular Systems” (July 2013)
Title of talk: “Path integral simulations of transport and dissipation: Vibrational instability in molecular rectifiers”
- University of Toronto, CQIQC-Fields Institute CQIQC-V Conference on Quantum Information and Quantum Control (Aug. 2013)
Title of talk: “Path integral simulations of transport and dissipation: vibrational instability in molecular rectifiers”.
- Bremen, Germany, CECAM workshop on nanophononics (Aug. 2013)
Title of talk: “Path integral simulations: Heat transfer in spin-bath models”
- Tel Aviv University, CECAM workshop on “Quantum Dynamics in Molecular and Nano-Materials: Mechanisms and Functionality” (Nov. 2013)
Title of talk: “Applications of influence functional path integral methodologies to charge and energy transfer problems”

- Telluride, Colorado, Workshop on Condensed Phase Dynamics (June 2014)
Title of talk: “Spin-boson model for heat transport problems”
- University of British Columbia, Conference on “Coherence and Control in the Quantum World: the Legacy of Moshe Shapiro” (Aug. 2014)
Title of talk: “From dissipative quantum dynamics to heat transfer at the nanoscale”
- Weizmann Institute of Science, Conference on “Coherence and Control in the Quantum World: Current and Future Trends” (Dec. 2014)
Title of talk: “Quantum dissipative dynamics and quantum transport: path integral formulation”
- Telluride, Colorado, Workshop on “Quantum effects in condensed-phase systems” (July 2015)
Title of talk: “Charge and energy transport at the nanoscale: Lessons from three simple models”
- University of Hong Kong, CECAM workshop: “Open Quantum Systems: Computational Methods” (Nov. 30 to Dec. 4 2015)
Title of talk: “Charge and heat transport at the nanoscale: elemental models, compound methods”
- San Sebastian, Spain, “Towards Reality in Modelling of Molecular Electronics” (June 12-16 2016)
Title of talk: Buttikers probes in molecular electronics: Applications to charge and heat transport”
- Telluride, Colorado, Workshop on “Condensed Phase Dynamics” (June 2016)
Title of talk: “From quantum dissipative dynamics to quantum transport: Full counting statistics”

11A. INVITED LECTURES

- University of Toronto, Condensed Matter Physics Seminar Series (November 2009)
- Tel Aviv University, Israel, Chemical Physics Seminar Program (December 2009)
- University of Pennsylvania, Physical Chemistry Seminar (November 2011)
- Department of Chemistry, University of Toronto, John Valteau Special Lecture -Colloquium, (November 2011)
- Department of Physics and Astronomy, Uppsala, Sweden, Seminar (May 2012)
- School of Chemistry, Tel Aviv University, Physical Chemistry Seminar (Dec. 2012)
- Department of Chemistry, Weizmann Institute of Science, Physical Chemistry Seminar (Dec. 2013)
- Department of Chemistry, UCSD, Physical Chemistry Seminar (Feb. 2014)
- Department of Chemistry, University of Pittsburgh (April 2015)
- Department of Chemistry, Tulane University, New Orleans (September 2015)
- Department of Physics, Bar-Ilan University, Israel (December 2015)

- Physics Department, McMaster University, Colloquium (November 2016)
- Institute for Theoretical Physics, Technical University Berlin, Eugene-Wigner-Colloquium (December 2016)

11B. OTHER INVITED TALKS April 2016-2017

- “Quantum non-equilibrium phenomena” at the International Institute of Physics (IIP), Natal, Brazil, June 6 to 17, 2016. (declined)
- Telluride workshop on “Thermal Transport at the Nanoscale”, Telluride, June 2016. (declined) a
- 2016 Canadian Symposium on Theoretical and Computational Chemistry (CSTCC), Regina, Saskatchewan, July 2016. (canceled)
- The 21st International Workshop on Quantum Systems in Chemistry, Physics, and Biology (QSCP-XXI), UBC, Vancouver July 2-9, 2016. (declined)
- ICTS Program on Open Quantum Systems, Bangalore, India, July 2017. (declined)
- Symposium on ”Physical Chemistry for Energy and Medicine Research”, ACS meeting, Galveston Texas, Nov 10-12 (declined).
- “Non-Markovianity and Strong Coupling Effects in Thermodynamics”, Bad Honnef Germany, April 10-13 2017 (declined)
- CECAM meeting on “Seeking synergy between dynamics and statistics for non-equilibrium quantum processes”, June 2017 (confirmed)
- Symposium on Chemical Physics, University of Waterloo, Nov. 2017 (accepted).
- Quantum Thermodynamics, ITAMP Harvard, Nov. 2017 (accepted).

D. LIST OF COURSES

12. A. UNDERGRADUATE COURSES

CHM 223S, Physical Chemistry: The Molecular Viewpoint	2017
CHM 135S, Chemistry: Physical Principles	2017
CHM 326F, Introductory Quantum Mechanics	2012
CHM 221S/225S/223S, Physical Chemistry: The Molecular Viewpoint	2012,2013,2015,2016
PHY 479Y, Undergraduate Research Project	2011-2012
CHM 499Y, Introduction to Research in Chemistry	2009-2010
CHM 423F, Applied Quantum Mechanics	2008-2010
CHM 139S, Chemistry: Physical Principles	2008-2010, 2012, 2015,2016
CHM 499Y, Introduction to Research in Chemistry	2008-2009
CHM 299Y, Research Opportunity	2008-2009

B. GRADUATE COURSES

CHM 1443F, Intermediate Quantum Mechanics	2014, 2016
CHM 1490Y, Physical Chemistry Seminar	2012-2013
CHM 1478, Quantum Mechanics for Physical Chemists	2009, 2011

C. THESIS SUPERVISION: Ph.D. STUDENTS

Roya Moghaddasi Fereidani	Mechanisms of energy transport in molecules	2016-
Hava Friedman	Path integral simulations of charge and energy transfer	2015-
Michael Kilgour	Molecular electronic conduction: principles and functionality	2014-
Salil Bedkihal	Quantum transport through double-dot Aharonov-Bohm interferometers	2010-2014
Yelena Simine (nee Nicolin)	Theory of charge transport through vibrating molecules	2009-2014
Claire Xue Yu	Energy transfer at the molecular scale: Open quantum systems methodologies	2008-2013

RESEARCH SUPERVISION: POSTDOCTORAL FELLOWS/SCIENTISTS

Bijay K. Agarwalla	Thermoelectricity of nanojunctions	2015-
Edward Taylor	Quantum bounds for quantum transport	2014-2015
Manas Kulkarni	Equilibration in closed quantum systems	2012
Savannah S. Garmon	Exceptional points in open quantum systems	2009-2012
Malay Bandyopadhyay	DNA bubble dynamics and energy transfer in nanoscale junctions	2009-2012
Yun Zhou	Heat engines and information theory	2008-2010
Lianao Wu (Scientist)	Quantum energy transfer at the nanoscale: fundamentals and applications	2008-2009

UNDERGRADUATE RESEARCH SUPERVISION

Anqi Mu	Quantum thermodynamics	CQIQC Summer Fellow 2017
Roman Korol	Molecular thermopower	CQIQC Summer Fellow 2017 Excellence Research Award 2016
Hyehwang Kim	Tunneling-hopping conduction in DNA	Chemistry Research Scholarship 2016
Nazim Boudjada	Spin dynamics and heat transport	CQIQC Summer Fellow 2014
Amro Dodin	Landau Zener transitions in open systems	NSERC USRA 2013
Wei Jia Chen	Thermoelectricity of molecular junctions	NSERC USRA 2013
Kunal Tiwari	Equilibration in interacting quantum systems	PHY 479Y 2011-2012
Pengcheng Dong	Heat capacity of nonlinear chains	CHM 499Y 2009-2010
Yelena Nicolin	Dimers diffusion on temperature gradients	CHM 499Y 2008-2009
Guillermo Toro Silvero	The damped-anharmonic oscillator	CHM 299Y 2008-2009

D. OTHER TEACHING and OUTREACH ACTIVITIES

Second annual "Ask a Laureate event"; Poster, Judge	2011, 2013
Science Rendezvous (demo preparation and management)	2012
Pueblo Science (Volunteer)	2012-2014

E. ADMINISTRATIVE POSITIONS

13. A. UNIVERSITY SERVICE

Department of Chemistry:	Information Technology and Cybersecurity committee, chair. (2015-)
	Progress Through the Ranks (PTR) Research Committee (2015)
	Undergraduate Studies Committee (2010-2013)

Colloquium Committee (2007-2010)
Graduate Student Committee (2007-2010)
Scinet (Computing) Local Resource Allocation Committee (2009-2010)

Outside the Chemistry Department: Dean's Working Group on Cyber Risk Mitigation (2015-)
Scinet Local Resource Allocation Committee (2010-2011)

PhD Committee Pascal Hogan-Lamarr, Physics, committee member (2016-)
Karen Morenz, Chemistry, committee member (2017-)
Philippe Green, Chemistry, committee member (2017-)
Markarita Gladikh, Chemistry, committee member (2016-)
Parisa Zareapour, Physics, voting member, final exam (2015)
Bryan Robertson, Chemistry, committee member (2014-)
Olivier Pare-Labrosse, Chemistry, committee member (2014-)
Cyrille Lavigne, Chemistry, committee member, (2014-) oral exam (2016)
Dan Sun, Physics, voting member, final exam (2014)
Peter Colberg, Chemistry, oral exam (2013)
Cathal Smyth, Physics, committee member (2013-2014)
Oliver MacLean, Chemistry, committee member, oral exam, (2013-)
Calvin Cheng, Chemistry, committee member (2013-) oral exam (2014)
Daniel Oblinsky, Chemistry, committee member (2012-2014)
Hoda Hossein, Chemistry, final exam (2012)
Yaser Khan, Chemistry, oral exam (2011-2013)
Samansa Maneshi, Physics, final exam (2010)
Ryan Field, Physics, committee member, oral, final (2009- 2016)
Ali Nassimi, Chemistry, oral exam (2008)
Hanif Bayat, Chemistry, oral exam (2008)
Gary Ilev, Chemistry, final exam (2008)
Robert Grunwald, Chemistry, final exam (2008)

Chair of Final Oral Exam:

Kyu-sung Hwang, Physics (2016)
Megan Hostetter, Materials Science and Engineering (2015)
Maygan McGuire, Chemical Engineering and Applied Chemistry (2014)
Ankur Saxena, Material Science and Engineering (2012)
Matthew Killi, Physics (2012)
So Takei, Physics (2008)
Sam Mavandadi, Electrical and Computer Engineering (2008)

Master Thesis: Reader Amro Dodin (2016)
Julia Endicott (2014)
Zaheen Sadeq (2012)
Jordan Pelc (2008)

13. B. OUTSIDE THE UNIVERSITY SERVICE

Journal Referee (~ 25 in 2015) APS, ACS, RSC, AIP, Elsevier and IOP Journals, AAAS including:
Phys. Rev., JCP, JPC, Science, PNAS, Nano Lett., PCCP,
Chemical Science, EPL, ACS Nano, Small, JAP, J. of Stat. Mech, NJP.
Ontario Graduate Scholarships: Member of adjudication panel (2012)
Conference Organization: -100th Canadian Chemistry Conference and Exhibition (2017),
Co-chair, PT division program

