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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:	dvira.segal@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 2017-	Professor, Department of Chemistry, University of Toronto
July 2012-2017	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

2014-2023	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 (CIC): Member
Quantum Transport and Thermodynamics Society (QTTS)

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 transport processes in condensed phases. This includes: (i) Formulation of 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 mechanisms, including single-molecule conduction, molecular thermoelectrics.

(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 particular realizations. 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 and in modeling molecular heat engines. This work connects with the fields of "quantum thermodynamics" and "nanophononics".

(c) **Quantum statistical mechanics.** We are interested in validating the heat exchange fluctuation theorem, quantifying violations of the second law, in strongly-coupled many-body quantum systems. By acquiring the cumulant generating function of nontrivial models we calculate the corresponding (quantum) heat current and its moments.

(d) **Finite time thermodynamics.** We are exploring 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.

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 (2004). (4 pages)

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 (2005). (4 pages)

11. D. Segal and A. Nitzan, Spin-boson thermal rectifier, Phys. Rev. Lett. **94**, 034301 (2005). (4 pages)

12. D. Segal and A. Nitzan, Heat rectification in molecular junctions, J. Chem. Phys. **122**, 194704 (2005). (12 pages)

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 (2005). (6 pages)

15. D. Segal, Thermoelectric effect in molecular junctions: A tool for revealing transport mechanisms, Phys. Rev. B **72**, 165426 (2005). (7 pages)

16. D. Segal and A. Nitzan, Molecular heat pump, Phys. Rev. E **73**, 026109 (2006). (9 pages)

17. D. Segal and M. Shapiro, Trapping of a single electron in a nanoscale Paul trap, Nano Lett. **6**, 1622-1626 (2006). (5 pages)

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). (4 pages)

19. D. Segal, Heat flow in nonlinear molecular junctions: Master equation analysis, Phys. Rev. B **73**, 205415 (2006). (9 pages)

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 (2007). (6 pages)

22. D. Segal, A. J. Millis, and D. R. Reichman, Non-equilibrium quantum dissipation in spin-fermion systems, Phys. Rev. B **76**, 195316 (2007). (21 pages)

23. D. Segal, Nonlinear thermal control in an N-terminal junction, Phys. Rev. E **77**, 021103 (2008). (6 pages)

24. D. Segal, Single mode heat rectifier: Controlling energy flow between electronic conductors, Phys. Rev. Lett. **100**, 105901 (2008). (4 pages)

25. D. Segal, Thermal conduction in molecular chains: Non-Markovian effects, J. Chem. Phys. **128**, 224710 (2008). (8 pages)

26. L.-A. Wu and D. Segal, Fourier's law of heat conduction: Quantum mechanical master equation analysis, Phys. Rev. E **77**, 060101(R) (2008). (4 pages)

27. D. Segal, Stochastic pumping of heat: Approaching the Carnot efficiency, Phys. Rev. Lett. **101**, 260601 (2008). (4 pages)

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 (2009). (4 pages)

30. L.-A. Wu and D. Segal, Sufficient conditions for thermal rectification in hybrid quantum structures, Phys. Rev. Lett. **102**, 095503 (2009). (4 pages)

31. L.-A. Wu, S. S. Wu, and D. Segal, Looking into DNA breathing dynamics via quantum physics, Phys. Rev. E **79**, 061901 (2009). (5 pages)

32. D. Segal, Vibrational relaxation in the Kubo oscillator: Stochastic pumping of heat, J. Chem. Phys. **130**, 134510 (2009). (10 pages)

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 (2009). (12 pages)

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). (5 pages)

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 (2010). (4 pages)

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). (4 pages)

37. Y. Zhou and D. Segal, Minimal model of a heat engine: An information theory approach, Phys. Rev. E **82**, 011120 (2010). (5 pages)

38. Y. Zhou and D. Segal, Interface effects in thermal conduction through molecular junctions: Numerical simulations, J. Chem. Phys. **133**, 094101 (2010). (9 pages)

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 (2010). (13 pages) Editors' Suggestion

40. L.-A. Wu and D. Segal, Quantum heat transfer: A Born-Oppenheimer method, Phys. Rev. E **83**, 051114 (2011). (5 pages)

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 (2011). (12 pages)

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). (9 pages) (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 (2011). (6 pages)

44. M. Bandyopadhyay and D. Segal, Quantum heat transfer in harmonic chains with self consistent reservoirs: Exact numerical simulations, Phys. Rev. E **84**, 011151 (2011). (8 pages)

45. L. Nicolin and D. Segal, Non-equilibrium spin-boson model: counting statistics and the heat exchange fluctuation theorem, J. Chem. Phys. **135**, 164106 (2011). (14 pages)

46. L. Nicolin and D. Segal, Quantum fluctuation theorem for heat exchange in the strong coupling regime, Phys. Rev. B **84**, 161414 (2011). (4 pages)

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 (2011). (13 pages)

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 (2012). (10 pages)

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). (15 pages)

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). (15 pages)

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). (5 pages)

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**, 261-275 (2013). (15 pages)

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). (28 pages)

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). (19 pages)

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 degenerate double-dot Aharonov-Bohm interferometers, Phys. Rev. B **87**, 045418 (2013). (12 pages)

57. D. Segal, Qubit-mediated energy transfer between thermal reservoirs: beyond Markovian Master equation, Phys. Rev. B **87**, 195436 (2013). (8 pages)

58. L. Simine and D. Segal, Path-integral simulations with fermionic and bosonic reservoirs: Transport and dissipation in molecular 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 (2013). (5 pages)

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). (14 pages)

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). (10 pages)

68. E. Taylor and D. Segal, Quantum bounds on heat transport through nanojunctions, Phys. Rev. Lett. **114**, 220401 (2015). (5 pages +supplementary)

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+ supplementary)

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) (11 pages) (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, 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). (12 pages)

83. R. Korol, M. Kilgour, and D. Segal, Thermopower of molecular junctions: Tunneling to hopping crossover in DNA, J. Chem. Phys. **145**, 224702 (2016). (9 pages).

84. H. Friedman, B. K. Agarwalla, and D. Segal, Effects of vibrational anharmonicity on molecular electronic conduction and thermoelectric efficiency, J. Chem. Phys. **146**, 092303 (2017). (16 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. **19**, 043030 (2017). (14 pages).

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). (9 pages).

87. 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, J. Chem. Phys. **147**, 054104 (2017). (8 pages)

88. B. K. Agarwalla, J.-H. Jiang, D. Segal, Quantum efficiency bound for continuous heat engines coupled to noncanonical reservoirs, Phys. Rev. B **96**, 104304 (2017). (6 pages)

89. A. Mu, B. K. Agarwalla, G. Schaller, D. Segal, Qubit absorption refrigerator at strong coupling, New J. Phys. **19**, 123034 (2017). (17 pages)

90. R. Korol, M. Kilgour, and D. Segal, ProbeZT: Simulation of transport coefficients of molecular electronic junctions under environmental effects using Buttiker's probes, Computer Physics Communications **224**, 396-404 (2018). (9 pages)

91. R. Korol and D. Segal, From exhaustive simulations to key principles in DNA nanoelectronics, J. Phys. Chem. C **122**, 8, 4206-4216 (2018). (11 pages)

92. D. Segal, Current fluctuations in quantum absorption refrigerators, Phys. Rev. E **97**, 052145 (2018). (9 pages) PRE Kaleidoscope

93. H. M. Friedman, B. K. Agarwalla, and D. Segal, Quantum energy exchange and refrigeration: A full-counting statistics approach, New J. Phys. **20**, 083026 (2018) (19 pages)

94. M. Kilgour and D. Segal, Coherence and decoherence in quantum absorption refrigerators, Phys. Rev. E **98**, 012117 (2018). (13 pages)

95. B. K. Agarwalla and D. Segal, Assessing the validity of the thermodynamic uncertainty relation in quantum systems, Phys. Rev. B **98**, 155438 (2018). (9 pages)

96. O. Shein Lumbroso, L. Simine, A. Nitzan, D. Segal, and O. Tal, Electronic noise due to temperature difference in atomic-scale junctions, Nature **562**, 240-244 (2018). (5 pages+ Supplementary Info).

97. J. Liu, C. Yu Hsieh, D. Segal, and G. Hanna, Heat transfer statistics in mixed quantum-classical systems, J. Chem. Phys. **149**, 224104 (2018). (13 pages)

98. N. Kalantar and D. Segal, On the relationship between the mean first-passage time and the steady state transfer rate in classical chains, J. Phys. Chem. C **123** 1021 (2019). (Abraham Nitzan Festschrift) (11 pages)

99. R. Moghaddasi Fereidani and D. Segal, Phononic heat transport in molecular junctions: quantum effects and vibrational mismatch, J. Chem. Phys. **150**, 024105 (2019). (13 pages)

100. M. Ghoussoub, M. Xia, P. Duchesne, D. Segal, and G. Ozin, Principles of Photothermal Gas-Phase Heterogeneous CO2 Catalysis, Energy and Environmental Science 12, 1122 (2019). (21 pages)

101. S. Garmon, K. Noba, G. Ordonez, and D. Segal, Non-Markovian dynamics revealed at the bound state in continuum, Phys. Rev. A **99**, 010102 (R) (2019). (6 pages + supplementary information)

102. M. Kilgour, B. K. Agarwalla, and D. Segal, Path-integral methodology and simulations of quantum thermal transport: Full counting statistics approach, J. Chem. Phys. **150**, 084111 (2019). (16 pages) Editor's pick (Special Topic on Dynamics of Open Quantum Systems)

103. R. Korol and D. Segal, Machine Learning Prediction of DNA Charge Transport, J. Phys. Chem. B **123**, 2801 (2019). (11 pages + supplementary information) Young Scientist Virtual Special Issue

104. J. Liu, D. Segal and G. Hanna, Hybrid quantum-classical simulation of quantum speed limits in open quantum systems, J. Phys. A: Math. Theor. **52**, 215301 (2019).

105. B. K Agarwalla, M. Kulkarni, and D. Segal, Photon statistics of a double quantum dot micromaser: Quantum treatment, Phys. Rev. B **100**, 035412 (2019). (12 pages)

106. J. Liu, D. Segal, and G. Hanna, A loss-free excitonic quantum battery, J. Phys. Chem. C **123**, 18303-18314 (2019). (12 pages)

107. J. Liu and D. Segal, Thermodynamic uncertainty relation in quantum thermoelectric junctions, Phys. Rev. E, **99**, 062141 (2019) (12 pages)

108. J. Liu and D. Segal, Interplay of direct and indirect charge transfer pathways in donor-bridge-acceptor systems, J. Phys. Chem. B **123**, 6099-6110 (2019). (12 pages)

109. A. Mu[a], O. Shein Lumbroso[a], O. Tal and D. Segal, (a=equal contribution) Origin of the anomalous electronic shot noise in atomic-scale junctions, J. Phys. Chem. C **123**, 23853-23862 (2019). (10 pages + supplementary information)

110. S. Saryal, H. Friedman, D. Segal, and B. K. Agarwalla, Thermodynamic uncertainty relation in thermal transport, Phys. Rev. E **100**, 042101 (2019) (10 pages)

111. H. Friedman and D. Segal, Cooling condition for multilevel quantum absorption refrigerators, Phys. Rev. E **100**, 062112 (2019). (11 pages)

112. J. Liu and D. Segal, Generalized input-output method to quantum transport junctions. I. General formulation, Phys. Rev. B **101**, 155406 (2020). (13 pages)

113. J. Liu and D. Segal, Generalized input-output method to quantum transport junctions. II. Applications, Phys. Rev. B **101**, 155407 (2020). (15 pages)

114. H. M. Friedman, B. K. Agarwalla, O. Shein-Lumbroso, O. Tal, and D. Segal, Thermodynamic uncertainty relation in atomic-scale quantum conductors, Phys. Rev. B **101**, 195423 (2020). Editors Suggestion. (8 pages)

115. S. Pal, S. Saryal, D. Segal, S. Mahesh, B. K. Agarwalla, Experimental study of the thermodynamic uncertainty relation Phys. Rev. Research **2**, 022044 (R) (2020). (6 pages)

116. J. Liu and D. Segal, Dissipation-engineering of nonreciprocal quantum dot circuits: An input-output approach, Phys. Rev. B **102**, 125416 (2020). (18 pages)

117. J. Liu and D. Segal Sharp negative differential resistance from vibrational mode softening in molecular junctions, Nano Letters **20**, 8, 6128–6134 (2020). (7 pages)

118. J. Liu, H.-T. Chen, and D. Segal, Quantum Nondemolition Photon Counting With a Hybrid Electromechanical Probe, Phys. Rev. A **102**, 061501(R) (2020). (7 pages)

119. N. Kalantar, B. K. Agarwalla and D. Segal, On the definitions and simulations of vibrational heat transport in nanojunctions, J. Chem. Phys. **153**, 174101 (2020). (15 pages)

120. J. Liu and D. Segal, Coherences and the thermodynamic uncertainty relation: Insights from quantum absorption refrigerators, Phys. Rev. E **103**, 032138 (2021) (15 pages)

121. L.-A. Wu and D. Segal, Hamiltonian Transformability, Fast Adiabatic Dynamics and Hidden Adiabaticity, Scientific Reports **11**, 4648 (2021). (5 pages)

122. J. Liu, D. Segal, and G. Hanna, Reply to the "Comment on 'Loss-Free Excitonic Quantum Battery'" J. Phys. Chem. C **125**, 7521-7522 (2021). (2 pages)

123. N. Kalantar, B. K. Agarwalla and D. Segal, Harmonic chains and the thermal diode effect, arXiv:2103.00046. Phys. Rev. E., in press.

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. Thanopulos, 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. N. Anto Sztrikacs and D. Segal, Strong coupling effects in quantum thermal transport with the reaction coordinate method, arXiv:2103.05670. Under review in New. J. Phys.
2. S. Saryal, M. Gerry, I. Khait, D. Segal, and B. K. Agarwalla, Universal Bounds on Fluctuations in Continuous Thermal Machines, arXiv:2103.13513. Under review in Phys. Rev. Lett.
3. J. Liu and D. Segal, Boosting quantum battery performance by structure engineering, arXiv:2104.06522. Under Review, Phys. Rev. Lett.

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

Over the past 5 years I had received invitations to present my work (invited speaker) in $\sim 6-8$ focused conferences, per year. I had accepted invitations and presented my work in the following meetings:

- National University of Singapore, Singapore, "Transmission of Information and Energy in Nonlinear and Complex Systems (TIENCS)" (May 2008).

- Helsinki University of Technology, Finland, Conference on "Micro and Nanocryogenics" (Aug. 2008).
- The 92nd Canadian Chemistry Conference and Exhibition, Hamilton, Ontario, Canada "Quantum Chemical Dynamics Symposium" (June 2009).
- Telluride, Colorado, Workshop on "Quantum Transport in Nanoscale Molecular System" (July 2009).
- UCSD, La Jolla, California, A meeting on "Optimization at a small scale" (July 2009).
- Stuttgart, Germany, International symposium "Quantum Thermodynamics: Energy and Information Flow at the Nano-Scale" (Sep. 2010).
- Erice, Sicily, Italy, "New trends in nonlinear dynamics: Heat control and thermo-electric efficiency" HEAT2010 (Oct. 2010).
- Snogeholm, Sweden, "Thermodynamics: Can macro learn from nano?" (May 2011).
- Telluride, Colorado, Workshop on "Chemistry and Dynamics in Complex Environments" (June 2011).
- Telluride, Colorado, Workshop on "Quantum Transport in Nanoscale Molecular Systems" (Aug. 2011).
- Hebrew University, Israel Institute for Advanced Studies, Jerusalem, Workshop on Molecular Electronics (July 2012).
- Telluride, Colorado, Workshop on "Quantum Transport in Nanoscale Molecular Systems" (July 2013).
- University of Toronto, CQIQC-Fields Institute CQIQC-V Conference on Quantum Information and Quantum Control (Aug. 2013).
- Bremen, Germany, CECAM workshop on nanophononics (Aug. 2013).
- Tel Aviv University, CECAM workshop on "Quantum Dynamics in Molecular and Nano-Materials: Mechanisms and Functionality" (Nov. 2013).
- Telluride, Colorado, Workshop on Condensed Phase Dynamics (June 2014).
- University of British Columbia, Conference on "Coherence and Control in the Quantum World: the Legacy of Moshe Shapiro" (Aug. 2014).
- Weizmann Institute of Science, Conference on "Coherence and Control in the Quantum World: Current and Future Trends" (Dec. 2014).
- Telluride, Colorado, Workshop on "Quantum effects in condensed-phase systems" (July 2015).
- University of Hong Kong, CECAM workshop: "Open Quantum Systems: Computational Methods" (Nov. 30 to Dec. 4 2015).
- San Sebastian, Spain, "Towards Reality in Modelling of Molecular Electronics" (June 2016).
- Telluride , Colorado, Workshop on "Condensed Phase Dynamics", (June 2016).
- Paris, France, CECAM meeting on "Seeking synergy between dynamics and statistics for non-equilibrium quantum processes", (June 2017).
- ITAMP, Harvard University, Cambridge MA, Workshop on Quantum Thermodynamics (Oct. 2017).
- Waterloo, Canada, Symposium on Chemical Physics (Nov. 2017).
- ACS March meeting, Symposium on "The Chemistry of Molecular Electronics" (March 2018).
- The 101 Canadian Chemistry Conference and Exhibition (CSC101), symposium on 'Assessing complex free energy surfaces from molecular simulations: From electronic structure to mesoscopic processes', Edmonton (May 2018).
- Telluride , Colorado, Workshop on "Condensed Phase Dynamics" (July 2018).
- School and Workshop on Quantum and Nano Thermodynamics, University of Uppsala, Sweden (Sep. 2018).
- CSC 2019, Quebec City: Symposium on 'Recent Developments in Quantum Molecular Dynamics Algorithms and Applications' (June 2019)
- Banff International Research Station Workshop on Charge and Energy Transfer Processes: Open Problems in Open Quantum Systems Aug. 2019 (co-organizer)
- QTD2020 – Conference on Quantum Thermodynamics, Barcelona, Spain (Virtual, Oct. 2020).

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 Valleau Special Lecture, (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).
- Colloquium, Department of Physics and Astronomy, McMaster University (Nov. 2016).
- Colloquium, Department of Physics, Technical University Berlin (Dec. 2016).
- Quarantine Thermodynamics virtual seminar series, Trinity College Dublin (May 2020).
- Department of Chemistry, UC Berkeley, Pitzer Center for Theoretical Chemistry (Virtual seminar, June 2020).
- Department of Applied Physics, University of Geneva (Virtual seminar, Nov. 2020).
- Greater Boston Area Theoretical Chemistry Lecture Series (Virtual, April 2021).

11B. INVITED LECTURES (May. 2021-)

- Colloquium, Center for Nonlinear Studies Los Alamos National Laboratory (May 2021).
- Workshop on Quantum Transport, Telluride Science Research Center (July 2021)
- ACS Fall meeting, symposium on Synthesizing Quantum Coherence (Aug. 2021).
- KITP Program and conference on Application for Transport and Efficient Energy Conversion in Quantum Systems (Santa Barbara, Aug 2021).
- American Conference on Theoretical Chemistry, Squaw Valley, CA, (July 2022)
- PacificChem Hawaii, Quantum coherence in energy transfer symposium (Dec. 2021)
- PacificChem Hawaii, Molecular Electronics: The synergy of synthesis, measurement and theory (Dec. 2021).
- WE-Heraeus-Seminar on Photon, Phonon, and Electron Transitions in Coupled Nanoscale Systems (Postponed from 2021 to 2022).

D. <u>LIST OF COURSES</u>

12. A. UNDERGRADUATE COURSES

CHM 427, Statistical Mechanics	2021
CHM 221/225/223S, Physical Chemistry: The Molecular Viewpoint	2012-2013, 2015-2020
PHY 472H, Supervised Readings II	2020
PHY 479Y, Undergraduate Research Project	2011-2012, 2017-2018
CHM 135/139S, Chemistry: Physical Principles	2008-2010, 2012, 2015-2019
CHM 326F, Introductory Quantum Mechanics	2012
CHM 423F, Applied Quantum Mechanics	2008-2010
CHM 499Y, Introduction to Research in Chemistry	2008-2010, 2019-2021
CHM 299Y, Research Opportunity	2008-2009

B. GRADUATE COURSES

CHM 1480S, Statistical Mechanics	2021
CHM 1443F, Intermediate Quantum Mechanics: Focus on open systems	2014, 2016, 2018
CHM 1490Y, Physical Chemistry Seminar	2012-2013
CHM 1478, Quantum Mechanics for Physical Chemists	2009, 2011

C. THESIS SUPERVISION: MSc and Ph.D. STUDENTS

Matthew Gerry	Thermodynamics uncertainty relation in quantum systems	2020-
Na'im Kalantar	Thermal rectification in classical chains	2020-
Francisco Lai-Liang	Spin filtering in chiral biomolecules	2020-
Nicholas Anto-Sztrikac	Reaction Coordinate method in quantum transport	2019-
Hava Friedman	Quantum transport and quantum thermodynamics	2015-2020
Roya Moghaddasi Fereidani	Energy transport in molecules	2016-2018
Michael Kilgour	Molecular conduction: From principles to functionality	2014-2019
Salil Bedkihal	Quantum transport in 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/RESEARCH ASSOCIATES

Ilia Khait	Machine learning techniques in quantum thermodynamics	2020-
Junjie Liu	Mixed quantum-classical simulations	2019-
Abhay Shastry	Flicker noise in atomic scale junctions	2018-2019
Bijay K. Agarwalla	Thermoelectricity of nanojunctions	2015-2017
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	Quantum energy transfer at the nanoscale: fundamentals and applications	2008-2009

UNDERGRADUATE RESEARCH SUPERVISION

Felix Ivander	Quantum transport at the nanoscale	CQIQC Summer Fellow 2021
Jiaming Wang	Thermal conduction in molecules	NSERC USRA 2019
Na'im Kalantar	Classical transport	NSERC USRA 2018, CQIQC 2019
Robert Adam Lang	Quantum absorption refrigerators	Summer 2018
Anqi Mu	Quantum thermodynamics	CQIQC Summer Fellow 2017
Roman Korol	Molecular thermopower	CQIQC Summer Fellow 2017 Excellence Research Award 2016-2018
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, Pueblo Science	2012-2014

E. ADMINISTRATIVE POSITIONS

13. A. UNIVERSITY SERVICE

Department of Chemistry:	Information Technology and Cyber security committee, chair. (2015-2018) Search Committees (2019, 2020) Building Oversight Committee (2020-) Departmental Advisory Committee (2020-) Promotions Committee (2020-) Undergraduate Studies Committee (2010-2013, 2018-2019) Progress Through the Ranks Research Committee (2015, 2018) Colloquium Committee (2007-2010, 2019-2020) Graduate Student Committee (2007-2010)
Outside the Chemistry Department:	Interim Director (April 2021 -), Centre for Quantum Information and Quantum Control (CQIQC) Dean's representative in Search Committees (2018-2019) Dean's Working Group on Cyber Risk Mitigation (2015-2017) Scinet Local Resource Allocation Committee (2010-2011)
PhD Committees:	Ongoing: ∼15 students from the Departments of Chemistry and Physics

13. B. OUTSIDE THE UNIVERSITY SERVICE

Journal Referee (∼ 20 in 2020)	APS, ACS, RSC, AIP, Elsevier and IOP Journals, AAAS including: Phys. Rev., JCP, JPC, JACS, Science, Nature, PNAS, Nano Lett., PCCP, Chemical Science, EPL, ACS Nano, Small, NJP.
Ontario Graduate Scholarships:	Member of adjudication panel (2012)
Guest Editor	Journal of Physical Chemistry A Abraham Nitzan Festchrift 2019 (with M. Galperin, J. Subotnik)
Conference Organization:	**(i)** Condensed Phases Dynamics (Telluride 2020, turned virtual) **(ii)** Banff International Research Station BIRS (2019), Co-organizer of the workshop "Charge and Energy Transfer Processes: Open Problems in Open Quantum Systems". **(iii)** Penn Conference in Theoretical Chemistry (PCTC) (2019) **(iv)** 100th Canadian Chemistry Conference and Exhibition (2017), Co-chair, PT division program (12 symposia) Co-organizer, Symposium on "Quantum Dynamics in Chemistry" **(v)** Theoretical Chemical Physics Symposium, 93rd Canadian Chemistry Conference and Exhibition (2010)
External Thesis Examiner	Physics, University of Bordeaux (2020) Physics, University of Konstanz (2019) Chemistry, University of British Columbia (2018) Physics, National University Singapore (2015) Physics, Raman Research Institute Bangalore (2009)
Grant and Fellowship Review (2007-2020)	NSF, DOE-BES, RCSA, BSF, Alfred P. Sloan Foundation, NSERC Discovery Grant, GIF, NWO, DFG, ISF, Research Corporation (Cortell) US Air Force (AFOSR), BSF, ISF, Ikerbasque foundation.