Barry D. Dunietz

Curriculum Vitae

(as of April, 2018)

Work Address

Department of Chemistry
Kent State University, Williams Hall
Kent, OH 44242
Phone: 330-672-2032;Fax: 330-672-3816;
email: bdunietz@kent.edu

Education

2000	**Ph.D**	Columbia University, New York (Chemical Physics)
1999	**M.Phill**	Columbia University, New York (Chemical Physics)
1994	**B.Sc.**	Tel-Aviv University, Israel (Chemistry major & Computer Science minor) Magna cum Laude

Academic Positions

2016– **Associate Professor of Chemistry**
Department of Chemistry, Kent State University, Kent, OH

2012–2016 **Assistant Professor of Chemistry**
Department of Chemistry, Kent State University, Kent, OH

2004–2012 **Assistant Professor of Chemistry**
Department of Chemistry, University of Michigan, Ann Arbor, MI

2001–2004 **Post Doctoral research scientist** with *Prof. M. Head-Gordon*
Department of Chemistry, University of California, Berkeley, CA

1995–2000 **Graduate student and research assistant** with *Prof. R. Friesner*
Department of Chemistry, Columbia University, New York, NY
Thesis topics:
a) Multi-configurational localized perturbation theory
b) Biological applications of quantum chemistry methodologies.

1994–1995 **Research assistant** with *Prof. U. Kaldor*
Chemistry Department, Tel-Aviv university, Israel.
Develop efficient code implementing coupled cluster method.

Teaching – Courses taught

Elementary Physical Chemistry (KSU)
Physical Chemistry I (KSU)
General Chemistry II, and Honors General Chemistry II (KSU)
Special Topics: Computational Chemistry (KSU)
Quantum Chemistry (UM)
Computational Chemistry Laboratory (UM)
Physical Chemistry I (UM)
General Chemistry: Macroscopic Investigations & Reaction Principles (UM)

Grants and Awards

- Currently funded research grants:
  - DOE/BES, 9/2017-9/2020: Lead PI, co-PIs Prof. Eitan Geva (Uni. of Michigan) and Prof. Margaret Cheung (Uni. of Houston)
    "Post-Marcus Theory and Simulation of Interfacial Charge Transfer Dynamics in Organic Semiconducting Materials" ($1,263,717)
  - NSF/CHEM, 7/2014-6/2018: Single PI
    "Charge transfer, injection and mobility in organic semi-conducting materials: modeling for insight on mechanistic aspects" ($330,000)
  - ICAM Postdoctoral Fellowship Award, 12/2015-12/2017: Lead PI, co-PI Prof Eitan Geva (Uni. of Michigan)
    "Ab-initio molecular modeling of electron transfer and transport in organic semiconductor crystals" ($50,000)
- Pending grants:
  - NSF/CHEM, 7/2018-6/2021: Single PI
    "Charge and Excitation Energy Transfer in the Photosynthetic Reaction Center: A first principles based perspective" (Proposed $300,000)
- Past funded grants:
  - DOE/BES, 9/2016-9/2017: Lead PI, co-PIs Prof. Eitan Geva (Uni. of Michigan) and Prof. Margaret Cheung (Uni. of Houston)
    "Post-Marcus Theory and Simulation of Interfacial Charge Transfer Dynamics in Organic Semiconducting Materials" ($270,000)
  - DOE/BES, 2010-2015: Single PI:
    "Electronic-structure modeling of electron transport switching in energy conversion schemes", ($406,000)

    9/2012-4/2016: Single PI
    "Electronic-structure modeling of electron transport switching in energy conversion schemes" ($203,000) (The funding of the second half of the same grant was executed at KSU.)
  - DOE/BES, 8/2009-7/2014: Co-PI in an Energy Frontier Research Center (EFRC), lead PI P. Green
    "Center for solar and thermal energy conversion in complex materials (CSTECCM)" ($19,500,000 for Center; $517,582 to Dunietz laboratory)

Publications

Peer Reviewed Publications:

1. C. McCleese, Z. Yu, N. N. Esemoto, C. Kolodziej, B Maiti, S Bhandari, B. D. Dunietz, C. Burda, and M. Ptaszek "Excitonic Interactions in Bacteriochlorin Homo-Dyads Enable Charge Transfer: A New Approach to the Artificial Photosynthetic Special Pair" , *J. Phys. Chem. B*, **122** (2018) 4131.

2. A. A. Kananenka, X. Sun, A. Schubert, B. D. Dunietz, and E. Geva "A Comparative Study of Different Methods for Calculating Electronic Transition Rates", *J. Chem. Phys.*, **148** (2018) 102304.

3. S. Bhandari, Z. Zheng, B. Maiti, C.-M. Chuang, M. Porel, Z.-Q. You, V. Ramamurthy, C. Burda, J. M. Herbert, and B. D. Dunietz "What Is the Optoelectronic Effect of the Capsule on the Guest Molecule in Aqueous Host/Guest Complexes? A Combined Computational and Spectroscopic Perspective", *J. Phys. Chem. C.*, **121** (2017) 15481-88.

4. B. Maiti, S. Sarkar, A. Schubert, S. Bhandari, K. Wang, Z. Li, R. J. Twieg, and B. D. Dunietz " Enhancing charge mobilities in organic semiconductors by selective fluorination: a design approach based on a quantum mechanical perspecitve", *Chem Sci.*, **8** (2017) 6947-53.

5. A. Yamada, Q. Feng, Q. Zhou, A. Hoskins, K. M. Lewis, and B. D. Dunietz "Conductance of Junctions with Acetyl-Functionalized Thiols: A First-Principles-Based Analysis", *J. Phys. Chem. C.*, **121** (2017) 10298-304.

6. Q. Zhou, A. Yamada, Q. Feng, A. Hoskins, A., B. D. Dunietz, and K. M. Lewis "Modification of molecular conductance by in-situ deprotection of thiol-based porphyrin", *ACS Appl. Mater. Interfaces*, **9** (2017) 15901-06.

7. B. Maiti, A. K. Manna, C. McCleese, T. L. Doane, S. Chakrapani, C. Burda, and B. D. Dunietz "Photoinduced Homolytic Bond Cleavage of the Central Si-C Bond in Porphyrinic Macrocycles Is a Charge Polarization Driven Process", *J. Phys. Chem. A.*, **120** (2016) 7634-40.

8. A. Yamada, Q. Feng, A. Hoskins, K. Fenk, and B. D. Dunietz "Achieving Predictive Description of Molecular Conductance by using a Range-Separated Hybrid Functional", *Nano. Lett.*, **16** (2016) 6092-98.

9. S. Sarkar, H. P. Hendrickson, D. Lee, F. DeVine, J. Jung, E. Geva, J. Kim, and B. D. Dunietz "Phosphorescence in Bromobenzaldehyde can be enhanced through intramolecular heavy atom effect", *J. Phys. Chem. C*, **121** (2017) 3771-77.

10. Q. Feng, Y. Atsushi, R. Baer, and B. D. Dunietz "Deleterious effects of exact exchange functionals on predictions of molecular conductance", *J. Chem. Theory Comput.*, **12** (2016) 3431-35.

11. M. H. Lee, E. Geva, and B. D. Dunietz "The Effect of Interfacial Geometry on Charge-Transfer States in the Phthalocyanine/Fullerene Organic Photovoltaic System", *J. Phys. Chem. A.*, **120** (2016) 2970-75.

12. A. K. Manna, D. Balamurugan, M. S. Cheung, and B. D. Dunietz "Unraveling the Mechanism of Photoinduced Charge Transfer in Carotenoid-Porphyrin-C_{60} Molecular Triad", *J. Phys. Chem. Lett.*, **6** (2015) 1231-37.

13. A. K. Manna, M. H. Lee, K. L. McMahon, and B. D. Dunietz "Calculating High Energy Charge Transfer States Using Optimally Tuned Range-Separated Hybrid Functionals", *J. Chem. Theo. Comp.*, **11** (2015) 1110-17.

14. D. E. Wilcox, M. H. Lee, M. E. Sykes, A. Niedringhaus, E. Geva, B. D. Dunietz M. Shtein, and J. P. Ogilvie "Ultrafast Charge-Transfer Dynamics at the Boron Subphthalocyanine Chloride/C_{60} Heterojunction: Comparison Between Experiment and Theory", *J. Phys. Chem. Lett.*, **6** (2015) 569-75.

15. Y. Shao, et al " Advances in molecular quantum chemistry contained in the Q-Chem 4 program package", *Mol. Phys.* **113** (2015) 184-215.

16. Z. Zheng, K. M. Manna, H. Phillips, M. Hammer, C. Song, E. Geva, and B. D. Dunietz "Molecular structure, spectroscopy and photo induced kinetics in tri-nuclear cyanide bridged complex in solution: A first principle perspective", *J. Amer. Chem. Soc.* **136** (2014) 16954-16957.

17. M. H. Lee, B. D. Dunietz, and E. Geva "Donor-to-donor vs. donor-to-acceptor interfacial charge transfer states in the phthalocyanine-fullerene organic photovoltaic system", *J. Phys. Chem. Lett.*, **5** (2014) 3810-16.

18. K. M. Manna, and B. D. Dunietz "Communication: Charge-transfer rate constants in zinc-porphyrin-porphyrin-derived dyads: A Fermi golden rule first-principles-based study", *J. Chem. Phys.* **141** (2014) 121102.

19. H. Phillips, Z. Zheng, and E. Geva, and B. D. Dunietz "Orbital Gap Predictions for Rational Design of Organic Photovoltaic Materials", *Opto Elect.*, **15** (2014) 1509-20.

20. M. H. Lee, B. D. Dunietz, and E. Geva "Calculation from First Principles of Golden-Rule Rate Constants for Photo-Induced Subphthalocyanine/Fullerene Interfacial Charge Transfer and Recombination in Organic Photovoltaic Cells", *J. Phys. Chem. C.*, **118** (2014) 9780-89.

21. M. H. Lee, B. D. Dunietz, and E. Geva "Calculation From First Principles of Intramolecular Golden-Rule Rate Constants for Photo-Induced Electron Transfer in Molecular Donor-Acceptor Systems", *J. Phys. Chem. C.*, **117** (2013) 23391.

22. M. H. Lee, and B. D. Dunietz "Active Control of Thermal Transport in Molecular spin valves", *Phys. Rev. B.* **88** (2013) 045421.

23. R. Balachandran, P. Reddy, B. D. Dunietz, and V. Gavini " End-group influence on frontier molecular orbital reorganization and thermoelectric properties of molecular junctions", *J. Phys. Chem. Lett.*, **4** (2013) 3825-33.

24. S. Zheng, E. Geva, and B. D. Dunietz " Solvated charge transfer states of functionalized anthracene and tetracyanoethylene dimers: A computational study based on a range separated hybrid functional and charge constrained self-consistent field with switching Gaussian polarized continuum models", *J. Chem. Theo. Comp.*, **9** (2013) 1125-31.

25. A. Tan, R. Balachandran, B. D. Dunietz, S.-Y. Jang, V. Gavini, and P. Reddy "Length Dependence of Frontier Orbital Alignment in Aromatic Molecular Junctions", *Appl. Phys. Lett.*, **101** (2012) 243107.

26. P. P. Pal, and B. D. Dunietz "On symmetry relationships for suppressing ghost transmission artifact and obtaining reliable transport modeling in molecular junction models", *J. Chem Phys.* , **137** (2012) 194104.

27. H. Phillips, E. Geva, and B. D. Dunietz "Examining Symmetry-Hidden Charge Transfer Excitations using Range-Separated Density Functionals", *J. Chem. Theo, Comp.*, **8** (2012) 2661-2668.

28. R. Balachandran, P. Reddy, B. D. Dunietz, and V. Gavini "End group induced charge transfer in molecular junctions: Effect on thermopower", *J. Phys. Chem. Lett.*, **3** (2012) 1962-67.

29. S. Zheng, H. Phillips, E. Geva, and B. D. Dunietz "*Ab-initio* study of the emissive charge-transfer states of solvated chromophore-functionalized silsesquioxanes", *J. Amer. Chem. Soc*, **134** (2012), 6944-47.

30. H. Phillips, S. Zheng, A. Hyla, R. Laine, T. Goodson III, E. Geva, and B. D. Dunietz "Ab-initio calculation of the electronic absorption of functionalized octahedral silsesquioxanes via time-dependent density functional theory with range separated hybrid functionals", *J. Phys. Chem. A.*, **116** (2012), 1137.

31. A. Tan, S. Sadat, J. Balchandran, V. Gavini, B. D. Dunietz, S.-Y. Jang, and P. Reddy "Effect of Length and Contact Chemistry on the Electronic Structure and Thermoelectric Properties of Molecular Junctions", *J. Amer. Chem. Soc.*, **133** (2011), 8838.

32. N. Sergueev, S. Seungha S., M. Kaviany, and B. D. Dunietz "Efficiency of thermoelectric energy conversion in biphenyl-dithiol junction: the effect of electron-phonon interaction", *Phys. Rev. B.*, **83,** , (2011), 195415.

33. H. Phillips, A. Prociuk, and B. D. Dunietz "Bias effects on the electronic spectrum of a molecular bridge", *J. Chem. Phys.*, **134** (2011), 54708.

34. Ding, B. and Washington V. and B. D. Dunietz "On the conditions for enhanced transport through molecular junctions based on metal centers ligated by pair of pyridazino-derived ligands", *Mol. Phys.*, **108** (2010), 2591.

35. A. Prociuk, and B. D. Dunietz "Photo-induced absolute negative current in a molecular electronic system", *Phys. Rev. B.*, **82**, (2010), 125449.

36. A. Prociuk, and H. Phillips, and B. D. Dunietz "Modeling transient aspects of coherehce-driven electron transport", *J. Phys.: Conf. Ser.* **220**, (2010), 012008.

37. T. Perrine, and B. D. Dunietz "Contact geometry symmetry dependence of field effect gating in single molecule transistors", *J. Amer. Chem. Soc.*, **132**, (2010), 2914.

38. C. Baiz, and S. J. Ledford, K. Kubarych, and B. D. Dunietz "Intermolecular Double Hydrogen-atom Transfer Reactions", *J. Phys. Chem. A.*, **113**, (2009), 4862.

39. A. Prociuk, and B. D. Dunietz "On the electronic spectra of a molecular bridge under non-equilibrium electric potential conditions", Chapter in Atomic and Molecular Systems, Dynamics, Spectroscopy, Clusters, and Nanostructures, **20**, (2009), 265.

40. M. Wong, B. Van-Kuiken, C. Buda, and B. D. Dunietz "Multi adsorption and Coadsorption of Hydrogen on model conjugated systems", *J. Phys. Chem. C.*, **113**, (2009), 12571.

41. T. M. Perrine, T. Berto, and B. D. Dunietz "Enhanced Conductance via Induced π-Stacking Interactions in Cobalt(II) Terpyridine Bridged Complexes", *J. Phys. Chem. B.* **112** (2008), 16070.

42. T. M. Perrine, and B. D. Dunietz "Conductance of a coblat(II) terpyridine complex based molecular transistor: A computational analysis", *J. Phys. Chem. A.*, **112**, (2008), 2043.

43. A. M. Geyer, E. S. Wiedner, J. B. Gary, R. L. Gdula, N. C. Kuhlmann, M. J. A. Johnson, B. D. Dunietz, and J. W. Kampf "Synthetic, mechanistic, and computational investigations of nitrile-alkyne cross-metathesis", *J. Amer. Chem. Soc.*, **130**, (2008), 8994-8999.

44. J. B. Gary, C. Buda,, M. J. A. Johnson, and B. D. Dunietz "Accessing metal-carbide chemistry - A computational analysis", *Organometallics*, **27**, (2008), 814-826.

45. Z. Zhao, and B. D. Dunietz "Ab initio study of charge transport of hydrogen functionalized palladium wires", *J. Chem. Phys.*, **129**, (2008), 024702.

46. T. M. Perrine, and R. G. Smith, C. Marsh, and B. D. Dunietz "Gating of single molecule transistors: Combining field-effect and chemical control", *J. Chem. Phys.*, **128**, (2008), 154706.

47. A. Prociuk, and B. D. Dunietz "Time-dependent current through electronic channel models using a mixed time-frequency solution of the equations of motion", *Phys. Rev. B.*, **78**, (2008), 165112.

48. M. Das, and B. D. Dunietz "Electron Transport through Heterogenous Intermolecular Tunnel Junctions", *J. Phys. Chem. C.*, **111**, (2007), 1535-1540.

49. T. M. Perrine, and B. D. Dunietz "Single molecule field effect transistors: A computational study of the effects of contact geometry and gating field orientation on conductance switching properties", *Phys. Rev. B.*, **75**, (2007), 195319.

50. T. M. Perrine, and B. D. Dunietz "Carbonyl mediated conductance through metal bound peptides; a computational study", *Nanotechnol*, **18** (2007), 424003.

51. C. R. Baiz, and B. D. Dunietz "Theoretical studies of conjugation effects on excited state intramolecular hydrogen-atom transfer reactions in model systems", *J. Phys. Chem. A.*, **111**, (2007), 10139-10143.

52. S. Kendler, G. R. Lambertus, B. D. Dunietz, , S. L. Coy, E. G. Nazarov, R. A. Miller, and R. D. Sacks "Fragmentation pathways and mechanisms of aromatic compounds in atmospheric pressure studied by GC-DMS and DMS-MS", *Inter. J. Mass. Spectro.*, **263**, (2007), 37-147.

53. A. Prociuk, and B. D. Dunietz "Benchmarking the performance of density functional theory based Green's function formalism utilizing different self-energy models in calculating electronic transmission through molecular systems", *J. Chem. Phys.*, **125**, (2006), 204717.

54. Y. Chen, A. Prociuk, T. M. Perrine, and B. D. Dunietz "Spin-dependent electronic transport through a porphyrin ring ligating an Fe(II) atom: An ab initio study", *Phys. Rev. B.*, **74**, (2006), 245320-9.

55. C. Buda, S. R. Caskey, M. J. A. Johnson, and B. D. Dunietz "Metathesis-enabled formation of a terminal Ru Carbide complex: A computational study", *Organometallics*, **25**, (2006), 4756-4762.

56. C. Buda, and B. D. Dunietz "Hydrogen Physisorption on the Organic Linker in Metal Organic Frameworks: Ab Initio Computational Study", *J. Phys. Chem B.*, **110**, (2006), 10479.

57. Y. Shao *et al*, "Advances in methods and algorithms in a modern quantum chemistry program package" *Phys. Chem. Chem. Phys.* **8** (2006), 3172.

58. B. D. Dunietz, N. Markovic, P. H. Ross, M. and Head-Gordon "Initiation of Electro-oxidation of CO on Pt based electrodes at full coverage conditions simulated by ab-initio electronic structure calculations", *J. Phys. Chem B.* **108**, (2004), 9888.

59. J. M. Ugalde, B. D. Dunietz, and A. Dreuw, and M. Head-Gordon, and R. J. Boyd "The spin dependence of spatial size of Fe(II) and of the structure of Fe(II)-porphyrins", *J. Phys. Chem A.*, **108**, (2004), 4653.

60. M. Head-Gordon, and T. Van Voorhis, G. J. O. Beran, and B. D. Dunietz "Local correlation models", (Chapter Book) *Computational Science - ICCS* **2660** (2003), 96.

61. C. Saravanan, B. D. Dunietz, and N. Markovic, G. Somorjai, M. Head-Gordon, and P. H. Ross "Electro-oxidation of CO on Pt electrodes simulated by electronic structure calculations" *J. Electroanal. Chem.* **554**, (2003), 459.

62. B. D. Dunietz, and M. Head-Gordon "Manifestations of symmetry breaking in self-consistent field electronic structure calculations" *J. Phys. Chem A.*, **107**, (2003), 9160.

63. B. D. Dunietz, and A. Dreuw, and M. Head-Gordon "Initial steps of the photodissociation of the CO ligated heme group", *J. Phys. Chem B.*, **107**, (2003), 5623.

64. B. D. Dunietz, and T. van Voorhis, and M. Head-Gordon "Geometric direct minimization of Hartree Fock calculations involving open shell wavefunctions with spin restricted orbitals", *J. Theo. Comp. Chem.*, **1**, (2002), 255.

65. A. Dreuw, and B. D. Dunietz, and M. Head-Gordon "Characterization of the relevant excited states in the photodissociation of the CO-ligated Hemoglobin and Myoglobin", *J. Amer Chem. Soc*, **124**, (2001), 12070.

66. B. D. Dunietz, and R. A. Friesner "Application and development of multiconfigurational localized perturbation theory", *J. Chem. Phys.* **115**, (2001), 11052.

67. B. F. Gherman, B. D. Dunietz, D. A. Whittington, S. J. Lippard, and R. A. Friesner "Activation of the C-H bond of methane by intermediate Q of methane monooxygenase: A theoretical study", *J. Amer Chem. Soc* **123**, (2001), 3836.

68. R. A. Friesner, and B. D. Dunietz "Large-scale ab-initio quantum chemical calculations on biological systems", *Acc. Chem. Res.* **34**, (2001), 351.

69. B. D. Dunietz, M. D. Beachy, Y. X. Cao, D. A. Whittington, S. J. Lippard, and R. A. Friesner "Large scale ab-initio quantum chemical calculation of the intermediate in the soluble methane monooxygenase catalytic cycle", *J. Amer Chem. Soc*, **122**, (2000), 2828.

70. R. A. Friesner, R. B. Murphy, M. D. Beachy, M. N. Ringnalda, W. T. Pollard, B. D. Dunietz, and Y. X. Cao "Correlated ab-initio electronic structure calculations for large molecules", *J. Phys. Chem. A.*, **103**, (1999), 1913.

71. B. D. Dunietz, R. B. Murphy, and R. A. Friesner "Calculation of atomization energies by a multiconfigurational localized perturbation theory - Application for closed shell cases", *J. Chem. Phys.*, **110**, (1999), 1921.

Presentations (since Fall 2006)

- Invited Lectures in Scientific Meetings
  - Materials Genome Initiative Principal Investigators Meeting NSF/DOE PI meeting "Post-Marcus theory and simulation of interfacial charge transfer dynamics in organic semiconductors", Betheshda, MD (March 2018)
  - American Chemical Society "Predictive description of photo-induced electron transfer or transport through molecular-resolved interfaces", New Orleans LA (March 2018)
  - TSRC workshop: Excited States: Electronic Structure and Dynamics, "First-principles based studies of photo-induced electron transfer and transport through molecular-resolved interfaces", Telluride, CO (July 2017)
  - TSRC workshop: Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy, "Predictive descriptions of voltage-biased or photo-induced processes through interfaces of molecular semi-conducting systems" , Telluride, CO (July 2017)
  - American Chemical Society "Spectroscopy and electron transfer processes in molecular systems of multi metal centers: Insight by ab-initio modeling", San Francisco, CA (April 2017).
  - Penn Conference in Theoretical Chemistry (PCTC) "Light Matter Interaction", Philadelphia, PA (August 2016).
  - Summer school on " Fundamentals on Organic Electronics", Case Western University, OH (July 2015).
  - TSRC Workshop "Nonequilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy", Telluride, CO (July 2015).
  - "24th Inter-American Photochemical Society Conference" Sarasota, FL (January 2015).
  - "Symposium on DFT and Charge Transfer" Weizmann Institute of Science, Israel (December 2014).
  - ESP2014: "2014 Conference on Excited States Processes." Sante Fe, NM (June, 2014).
  - Flagship CECAM workshop: "Quantum Dynamics in Molecular and Nano-Materials: Mechanisms and Functionality." Tel Aviv, Israel (November 2013).
  - 2013 Southeastern Regional Meeting of the American Chemical Society (SERMACS): "Electronic Structure in Complex Environments", Atlanta, GA (November 2013).
  - Gordon research conference on Time Dependent Density Functional Theory (invited discussion leader), Biddeford, ME (August 2013)
  - TSRC Workshop "Quantum Transport in Nanoscale Molecular Systems", Telluride, CO (July 2013).
  - 2nd Annual Symposium on Advances in Organic Photovoltaics, Kent state university, Kent, OH (April 2013)
  - American Physical Society, (invited session chair and speaker) Focus session on "DFT II: Molecular Conductance; Charge Transfer" Boston, MA (March 2012)
  - Gordon research conference on time dependent density functional theory (invited session chair and speaker), Biddeford, ME (August 2011)

- TSRC workshop "Computational molecular electronics", Telluride, CO (August 2011)
- Workshop on Simulation and Modeling of Emerging Electronics, Hong-Kong, China (Dec. 2010)
- An International Conference in Honor of Professor Henry F. Schaefer III, Berkeley, CA (May 2010)
- "Theoretical, Computational, and Experimental Challenges to Exploring Coherent Quantum Dynamics in Complex Many-Body Systems", Dublin, Ireland; (May 2010)
- "Quantum transport and dynamics in materials and biosystems: From molecular mechanisms to mesoscopic functionality", Dublin, Ireland; (May 2010)
- NSF workshop on progress in physical organic chemistry, Austin, TX (January 2010)
- "Progress in Non-Equilibrium Green's Function (PNEGF) workshop", Glassgow, Scotland (August 2009)
- TSRC Workshop "Computational molecular electronics", Telluride, CO (July 2009)
- APS: Focus session on computational molecular electronics (March 2009)
- International Society for Theoretical Chemical Physics (ISTCP)-VI, Vancouver (July 2008)
- Thirteenth International Workshop on quantum systems in chemistry and physics QSCP-XIII, Lansing, MI (July 2008)
- The Gentner-Minarva Time-Dependent Density-Functional-Theory symposium; Eilat, Israel (December 07)
- Lester Fest Symposium, Berkeley, CA (March 2007)

- Contributed Lectures in Scientific Meetings
  - ACS Goddard fest; Boston, MA (August 07)
  - APS " Transport through nanostructures" session; Denver, CO (March 07)
  - ACS special "hydrogen storage material" session; San Francisco, CA (Sept. 06)
  - TDDFT Workshop; Benasque, Spain August 06 (presented a poster)
  - ACS "Molecular electronics" session; Atlanta, GA (March 06)
  - American Computational and Theoretical Chemistry (ACTC); UCLA, CA (July 05); (presented two posters)

- Conference Chair and Organizer
  - American Physical Society; Boston MA (March 12) Session chair: "Focus Session: DFT V: Partitioning and Embedding Theories; Finite-Temperature".
  - Gordon research conference on time dependent density functional theory, Biddeford, ME (August 11), session chair.
  - American Computational and Theoretical Chemistry (ACTC); Northwestern University, Chicago, IL (July 08) Session chair.
  - 40th Midwest Theoretical Chemistry Conference (June 08). Co-organizer with Prof. E. Geva.

  - APS - "Transport through nanostructures" session; Denver, CO (March 07). Co-organizing with prof. Hongkun Park.

- Departmental seminars
  - Youngstown State University, Chemistry, Youngstown, OH (February 17)
  - Kent State University, Chemistry, Kent, OH (February 15)
  - Los Alamos National laboratory, NM (May 14)
  - Wright State University, OH (December 13)
  - Weizmann Institute of Science, Materials Science and Physical Chemistry departments, Tel-Aviv, Israel (July 13)
  - Houston University, Physics, Houston, TX (April 13)
  - Liquid crystal institute, Kent state university, Kent, OH (March 13)
  - Wayne state university, Detroit, MI (April 12)
  - Oakland university, MI (April 12)
  - Kent State university, Kent, OH (March 12)
  - Pacific Northwest National Laboratory (March 12)
  - University of Maryand, Baltimore County, Physics department (March 12)
  - Rutgers University, Newark, NJ (December 11)
  - Michigan State University, MI (March 11)
  - University of Northern Texas, TX (February 11)
  - Bowling Green State University, OH (December 10)
  - Bar-Ilan University, Ramat-Gan, Israel (November 09)
  - The Technion, Haifa, Israel (November 09)
  - Tel-Aviv University, Tel-Aviv, Israel (November 09)
  - Ben-Gurion University, Beer-Sheva, Israel (November 09)
  - Columbia University (November 09)
  - Boston University; Greater Boston theoretical chemistry seminars (October 09)
  - Harvard Uni; Greater Boston theoretical chemistry seminars (October 09)
  - M.I.T, Cambridge; Greater Boston theoretical chemistry seminars (October 09)
  - University of Washington, Seattle (May 09)
  - Georgia Tech (May 09)
  - University of Wisconsin at Madison; Material engineering seminars (March 09)
  - University of Southern California (February 09)
  - University California at LA (February 09)
  - University California at Irvine (February 09)
  - Indiana University at Bloomington (January 09)
  - Notredam university (January 09)
  - Ohio State (November 08)

  - Hebrew University, Jerusalem, Israel (October 08)
  - Wayne State University (October 08)
  - University of Arizona (Sept. 08)
  - University of Georgia (August 08)
  - University of Florida at Gainsville (April 08)
  - University of Wisconsin at Madison (March 08)
  - Rochester University (March 08)
  - Cornell University (March 08)
  - Northwestern University (January 08)
  - Michigan State University (Sept. 07)
  - Central Michigan University (December 06)
  - Western Michigan University (November 06)
  - Oakland University (05)

- Invitations Declined
  - WUN-SPintronics 2010 and the Materials Computation Summer School, University of Illinois (June 10).

Research Group Members

- Current Postdoctoral Fellows

  Sunandan Sarkar (since Dec. 2015)

  Alex Schubert (since 01/16 ICAM fellow, co-mentored with Prof. Geva [UM])

  Huseyin Aksu (since Jan. 2018)

  Ariela Kaspi (since Jan. 2018)

- Current Graduate Students (Research Assistants)

  Srijana Bhandari

  Bishnu Pant

- Former Postdoctoral Fellows

  Dr. Atsushi Yamada (08/15 - 01/17). Professor at Dept. Applied Molecular Chemistry; Kyushu University Center of Future Chemistry

  Dr. Qingguo Feng (09/14 - 12/15)

  Dr. Buddhadev Maiti (10/14- 11/15)

  Dr. Arun K Manna (01/13-11/14) Research fellow at Weizman Institure of Science, Israel.

  Dr. Myeong Lee. Research Post Doc (11/12-07/14). Research fellow at the University of Warwick, United Kingdom.

  Dr Zilong Zheng Post Doc (03/13-07/14). Research fellow at Georgia Institute of Technology.

Dr. Parta Pal: Research Post Doc (05/11-07/12). Research fellow at Northwestern University.

Dr. Shauhui Zheng: Research Post Doc (05/10-07/12). Research fellow at University of Washington.

Dr. Nikolai Sergueev: Research Post Doc (01/10-05/11). Research scientist at university of southern Carolina.

Dr. Trilisa Perrine: Faculty Development Post Doc (08/05-08/08). Faculty at Ohio Northern University.

Dr. Zhen Zhao: Research Post Doc (1/07-12/07).

Dr. Mousumi Das: Research Post Doc (10/05-9/06).

Dr. Corneliu Buda: Research Post Doc (11/04-9/06). Research scientist at the university of Virginia.

Dr. Yunqing Chen: Research Post Doc (12/04-4/05). Working at NVidia as a hardware engineer.

- Former Graduate Students

  Dr. Heidi Phillips (Chemistry, UM, 04/2015)

  Dr. Alexander Prociuk (Physics, UM, 08/2009)

- Rotation (visiting) Graduate Students

  Ms. Jessica Donheue (Winter 09)
  Ms. Surma Talapatra (Fall 09)
  Mr. Tim Berto (Winter 08)
  Mr. Brannon Gary (Fall 06)
  Ms. Miri Shlomi (Fall 05)
  Ms. Bei Ding (Winter 09)
  Mr. Sung Hei (Fall 08)
  Mr. Carlos Baiz (Winter 07)
  Mr. Ron Smith (Winter 06)

- Former Undergraduate Research Students

  Mr. Austin Hoskins (HS)
  Ms. Francis Devine
  Mr. Jacob Smith
  Ms. Francis Devine
  Mr. Robert Liu
  Ms. Sarah Ledford
  Mr. Ben Van Kuiken
  Ms. Jessica Shost
  Ms. Vicotria Washington
  Mr. Alexander Hyla
  Mr. Tatsuya Kamiya
  Mr. Miguel Wong
  Mr. Christopher Lee Marsh

Service

- Departmental Service

  Faculty search committees analytical and cphysical chemistry

  Graduate studies and admission committee

  Recruitment committee

- University Service

  Reviewer for university seed projects

  Served on several graduate student dissertation committees (physics, applied physics and engineering programs)

- Graduate Student Dissertation Committees

  Bei Ding (UM/Chemistry, Chen)
  Seungha Shih (UM/Mechanical engineering, Kaviany)
  Randall Breckon (KSU/Chemistry, Twieg)
  Brannon Gary (UM/Chemistry, Sanford)
  Changgua Zhen (UM/Material Science and Engineering, Kieffer)
  Carlos Baiz (UM/Chemistry, Kubarych)
  Michael Orozco (UM/Chemistry, Sension)
  Frank Vazquez (UM/Chemistry, Geva)
  Henry Boateng (UM/Mathematics, Krasny)
  William Fisher (UM/Applied Physics, Rand)
  Meng Guo (UM/Chemistry, Goodson)
  John Hensslor (UM/Chemistry, Matzger)
  Damian Khan (UM/Applied Physics, Orr).
  Yunqing Chen (UM/Physics, Banaszak Holl and Orr)
  Chenyue Xing (UM/Chemistry, Andricioaei)

- Wide research community Service

  Co-organizer of a seminar series for "Computational and theoretical molecular physics" funded by the Michigan center for theoretical physics (MCTP) (years 2008-2010)

  Co-organizer of the 40th Midwest Theoretical Chemistry Conference (June 08)

  Co-organizing with Prof. Hongkun Park from Harvard University a focus session on "Electron Transport in Nanostructures" in the APS national March 07 meeting.

- Manuscript Reviewer for the Following Journals:

  Biochemistry
  Chemical Physics Letters
  Journal of the American Chemical Society
  Journal of Chemical Physics
  Journal of Computational Chemistry
  Journal of Physical Chemistry
  Nano Letters
  Nature Nanotechnology
  Physical Review B
  Physical Review Letters
  Proceedings of the National Academy of Sciences of the USA
  Theoretical Chemistry Accounts
  Organometallics

- Grant Proposal Reviewer for the Following Agencies:

US department of energy (DOE), Basic Energy Sciences (BES) and National Energy Technology Laboratoryi (NETL).

Israel Science Foundation (ISF).

National Science Foundation (NSF)

Petroleum Research Fund (PRF)