Barry D. Dunietz

Curriculum Vitae

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Work Address

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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

2024–	**Professor of Chemistry**
2023	**Visiting Professor** Department of Molecular Chemistry and Materials Science, Weizmann Institute of Science, Rehovot, Israel
2016–2024	**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

Fundamentals of Chemistry (KSU)
Elementary Physical Chemistry Lab. (KSU)
Physical Chemistry I (KSU)
General Chemistry II, and Honors General Chemistry II (KSU)
†Computational Chemistry (Graduate level KSU)
†Practical Computational Chemistry (senior/elective KSU)
†Principles of Applied Physical Chemistry (Master's Program KSU)
Quantum Chemistry (UM)
Computational Chemistry Laboratory (UM)
Physical Chemistry I (UM)
General Chemistry: Macroscopic Investigations & Reaction Principles (UM)
† marks courses developed by Prof. Dunietz

Grants and Awards

- Currently funded research grants:
  - Department of Energy, Basic Energy Sciences, 09/2024-08/2027: Lead PI. Co PIs: Eitan Geva (University of Michigan), Margaret Cheung (PNNL) "Simulating Photo-Induced Electronic Energy and Charge Transfer Dynamics in Complex Molecular Systems and Their Spectroscopic Signature" ($862,477)
  - National Science Foundation, 01/2023-12/2025: Co-PI, Lead PI: Qiang Guan. "OAC Core: Interpretable Resilience Analysis Platform for Scientific Workflow Applications" ($574,640)
  - National Science Foundation, 11/2022-10/2025: Co-PI, Lead PI: Qiang Guan. "CyberTraining: Implementation: Small: Interactive and Integrated Training for Quantum Application Developers across Platforms" ($500,000)
- Pending grants:
  - National Science Foundation, 09/2025-08/2028: Single PI. " A Polarizable Consistent and Highly Effective Framework to Study Charge and Excitation Energy Transfer in Photosynthetic Reaction Centers: A First-principles Based Perspective" ($536,553) (Submitted 01/2024)
  - National Science Foundation, 06/2025-05/2028: Co-PI, Lead PI: Qiang Guan. "Collaborative Research: CS2: Verifiable Soft Error Correction for Exascale Scientific Computing." ($309,727) (Submitted 08/2024)
- Past funded grants:
  - DOE/BES, 9/2017-9/2022: 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, 7/2014-6/2019: Single PI
    "Charge transfer, injection and mobility in organic semi-conducting materials: modeling for insight on mechanistic aspects" ($325,683)

- KSU seed funding award 11/2017-11/2018: Single PI
  "Computational Design of New-Generation Metal-Based Molecular Anticancer Drugs" ($10,000)
- ICAM Postdoctoral Fellowship Award, 12/2015-12/2017: Lead PI, to fund a fellowship of a collaborative mentorship with Prof. Eitan Geva (Uni. of Michigan)
  "Ab-initio molecular modeling of electron transfer and transport in organic semiconductor crystals" ($50,000)
- 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. Khadiza Begam, Huseyin Aksu, Barry D Dunietz "Antioxidative Triplet Excitation Energy Transfer in Bacterial Reaction Center Using a Screened Range Separated Hybrid Functional" *J. Phys. Chem. B.* **128** (2024) 4315–4324

2. Alexander Schubert, Srijana Bhandari, Eitan Geva, and Barry D. Dunietz "A Computational Study of the Electronic Energy and Charge Transfer Rates and Pathways in the Tetraphenyldibenzoperiflanthene/Fullerene Interfacial Dyad" *J. Phys. Chem. Lett.* **14** (2023) 9569–9583

3. R Khatri, BD Dunietz Rapid communication: "Polarization consistent dielectric screening in polarizable continuum model calculations of solvation energies" *J. Chem. Phys.* **159** (2023) 071103

4. Amarasooriya MDS Jayawardhana, Srijana Bhandari, Ariela W Kaspi-Kaneti, Man Kshetri, Zihan Qiu, May Cheline, Hao Shen, Barry D Dunietz, Yao-Rong Zheng "Visible light-activatable platinum (IV) prodrugs harnessing CD36 for ovarian cancer therapy" *Dalton Transactions* **52** (2023) 10942-10950

5. Sloane Evariste, Alexandra M Harrison, Sunandan Sarkar, Arnold L Rheingold, Barry D Dunietz, Joachim W Heinicke, Emalyn Delgado Rosario, Sungwoon Yoon, Thomas S Teets, John D Protasiewicz "Luminescent 1 H-1, 3-benzazaphospholes" *RSC Adv.* **13** (2023) 594-601

6. Sara Ansteatt, Brian Uthe, Bikash Mandal, Rachel Gelfand, Barry D. Dunietz, Matthew Pelton, and Marcin Ptaszek "Engineering giant excitonic coupling in bioinspired, covalently bridged BODIPY dyads" *Phys. Chem. Chem. Phys.* **25** (2023) 8013-8027.

7. Bikash Mandal and Barry D. Dunietz "Effects of Solvent Dielectric on Thermally Activated Delayed Fluorescence: A Predictive Computational Polarization Consistent Approach" *J. Phys. Chem. A.* **127** (2022) 216-223.

8. Khadiza Begam, Gil Goobes, and Barry D. Dunietz "Solvent Dependent Nuclear Magnetic Resonance Molecular Parameters Based on a Polarization Consistent Screened Range Separated Hybrid Density Functional Theory Framework" *J. Chem. Theory Comput.* **18** (2022) 5259-5266.

9. Chandrima Chakravarty, Huseyin Aksu, Jessica Andrea Martinez Bernal, Pablo Ramos, Michele Pavanello, and Barry D. Dunietz "Role of Dielectric Screening in Calculating Excited States of Solvated Azobenzene: A Benchmark Study Comparing Quantum Embedding and Polarizable Continuum Model for Representing the Solvent" *J. Phys. Chem. Lett.* **13** (2022) 4849.

10. J. Tinnin, S Bhandari, P Zhang, E Geva, B. D. Dunietz, X Sun, M. S. Cheung "Correlating Interfacial Charge Transfer Rates with Interfacial Molecular Structure in the Tetraphenyldibenzoperiflanthene/C70 Organic Photovoltaic System" *J. Phys. Chem. Lett.*, **13** (2022) 763.

11. S Sarkar, P Durairaj, J. D. Protasiewicz, B. D. Dunietz "Enhancing fluorescence and lowering the optical gap through CP doping of a pi-conjugated molecular backbone: A computational-based design approach" *J. Photochem. Photobio.*, **8** (2021) 100089.

12. C. Chakravarty, H. Aksu, B. Maiti, and B. D. Dunietz "Electronic Spectra of C60 Films Using Screened Range Separated Hybrid Functionals" *J Phys. Chem. A.* , **125** (2021) 7625.

13. E Epifanovsky et al "Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package" *J. Chem. Phys.*, **155** (2021) 084801.

14. S. Bhandari, S. Sarkar, A. Schubert, A. Yamada, J. Payne, M. Ptaszek, E. Geva, B. D. Dunietz "Intersystem Crossing in Tetrapyrrolic Macrocycles. A First Principles Analysis" *J Phys. Chem. C.* , **125** (2021) 13493.

15. J. Tinnin, H. Aksu, Z. Tong, P. Zhang, E. Geva, B. D. Dunietz, X. Sun, and M. Cheung "CTRAMER: An open-source software package for correlating interfacial charge transfer rate constants with donor/acceptor geometries in organic photovoltaic materials" *J. Chem. Phys.*, **154** (2021) 214108.

16. E. Mulvihill, K. M. Lenn, X. Gao,, A. Schubert, B. D. Dunietz, and E. Geva "Simulating Energy Transfer Dynamics in the Fenna-Matthews-Olson Complex via the Modified Generalized Quantum Master Equation" *J. Chem. Phys.* , **154** (2021), 204109

17. D. Brian, Z. Liu, B. D. Dunietz, E. Geva, X. Sun "Three-state harmonic models for photoinduced charge transfer" *J. Chem. Phys.*, **154** (2021), 174105.

18. A. Goker, H. Aksu, B. D. Dunietz, "Heat flow enhancement in a nanoscale plasmonic junction induced by Kondo resonances and electron-phonon coupling" *Physica E: Low-dimensional Systems and Nanostructures*, **127** (2021) 114536.

19. A. W. Kaspi-Kaneti, S. Bhandari, A. Schubert, S. Huang, B. D. Dunietz "Cyanide Bridged Platinum-Iron Complexes as Cisplatin Prodrug Systems: Design and Computational Study" *ChemPhysChem*, **22** (2021) 106-111.

20. S. Bhandari, A. Yamada, A. Hoskins, J. Payne, H. Aksu, B. D. Dunietz "Achieving Predictive Description of Negative Differential Resistance in Molecular Junctions Using a Range-Separated Hybrid Functional" *Adv. Theory Simul.*, **4** (2021) 2000016.

21. Z. Hu, Z. Tong, M. S. Cheung, B. D. Dunietz, E. Geva, X. Sun "Photoinduced Charge Transfer Dynamics in the Carotenoid–Porphyrin–C60 Triad via the Linearized Semiclassical Nonequilibrium Fermi's Golden Rule" *J. Phys. Chem. B.*, **24** (2020) 9579.

22. H. Aksu, B. Maiti, B. M. Ptaszek, B. D. Dunietz "Photoinduced Charge Transfer in Zn(II) and Au(III)-Ligated Symmetric and Asymmetric Bacteriochlorin Dyads: A Computational Study" *J. Chem. Phys.*, **153** (2020) 134111.

23. J. Han, P. Zhang, H. Aksu, B. Maiti, X. Sun, E. Geva, B. D. Dunietz, M. S. Cheung "On the Interplay Between Electronic Structure and Polarizable Force Fields When Calculating Solution-Phase Charge Transfer Rates" *J. Chem. Theo. Comput.*, **16** (2020) 6481.

24. H. Aksu, S. K. Paul, J. M. Herbert, and B. D. Dunietz "How Well Does a Solvated Octa-acid Capsule Shield the Embedded Chromophore? A Computational Analysis Based on an Anisotropic Dielectric Continuum Model" *J. Phys. Chem. B.*, **124** (2020) 6998.

25. Z. Tong, X. Gao, M. S. Cheung, B. D. Dunietz, E. Geva, X. Sun "Charge Transfer Rate Constants for the Carotenoid-Porphyrin-C60 Molecular Triad Dissolved in Tetrahydrofuran: The Spin-Boson Model vs the Linearized Semiclassical Approximation" *J. Chem. Phys.*, **153** (2020) 044105.

26. J. Tinnin, S. Bhandari, P. Zhang, H. Aksu, B. Maiti, E. Geva, B. D. Dunietz, X. Sun, M. S. Cheung "Molecular-Level Exploration of the Structure-Function Relations Underlying Interfacial Charge Transfer in the Subphthalocyanine/C_{60} Organic Photovoltaic System" *Phys. Rev. Applied*, **13** (2020) 054075.

27. K. Begam, S. Bhandari, B. Maiti, B. D. Dunietz "Screened Range-Separated Hybrid Functional with Polarizable Continuum Model Overcomes Challenges in Describing Triplet Excitations in the Condensed Phase Using TDDFT" *J. Chem. Theo. Comput.*, **16** (2020) 3287.

28. I. A. MacKenzie, L. Wang, N. P. R. Onuska, O. F. Williams, K. Begam, A. M. Moran, B. D. Dunietz, D. A. Nicewicz "Discovery and characterization of an acridine radical photoreductant" *Nature*, **580** (2020) 76-80.

29. B. Maiti, Kunlun Wang, S. D. Bunge, R. J. Twieg and B. D. Dunietz "Enhancing charge mobilities in self-assembled N-I halogen bonded organic semiconductors: A design approach based on experimental and computational perspectives " *Org. Electron.*, **79** (2020) 105637.

30. H. Aksu, A. Schubert, S. Bhandari, A. Yamada, E. Geva, B. D. Dunietz "On the Role of the Special Pair in Photosystems as a Charge Transfer Rectifier" *J. Phys. Chem. B.*, **124** (2020) 1987-1994.

31. Y. Song, A. Schubert, X. Liu, S. Bhandari, S. R. Forrest, B. D. Dunietz, E. Geva "Efficient Charge Generation via Hole Transfer in Dilute Organic Donor–Fullerene Blends" *J. Phys. Chem. Lett.*, **11** (2020) 2203-2210.

32. H. Aksu, A Schubert, E. Geva, B. D. Dunietz "Explaining Spectral Asymmetries and Excitonic Characters of the Core Pigment Pairs in the Bacterial Reaction Center using Screened Range-Separated Hybrid Functionals" *J. Phys. Chem. B.*, **123** (2019) 8970.

33. E. Mulvihill, X. Gao, Y. Liu, A. Schubert, B. D. Dunietz, and E. Geva "Combining the Mapping Hamiltonian Linearized Semiclassical Approach with the Generalized Quantum Master Equation to Simulate Electronically Nonadiabatic Molecular Dynamics" *J. Chem. Phys.*, **151** (2019) 074103.

34. S. Bhandari, B. D. Dunietz "Quantitative accuracy in calculating charge transfer state energies in solvated molecular dimers using screened range separated hybrid functional within a polarized continuum model" *J. Chem. Theory Comput.*, **15** (2019) 4305.

35. E. Mulvihill, A. Schubert, X. Sun, B. D. Dunietz, and E. Geva "A modified generalized quantum master equation for simulating electronically nonadiabatic dynamics" *J. Chem. Phys.*, **150** (2019) 034101.

36. Y. Song, and A. Schubert, and E. Maret, and R. K. Burdick, and B. D. Dunietz and E. Geva, and J. P. Ogilvie "Vibronic structure of photosynthetic pigments probed by polarized two-dimensional electronic spectroscopy and ab initio calculations" *Chem. Sci.*, **10** (2019) 8143.

37. B. Maiti, K. Wang, S. Bhandari, S. Bunge, R. J. Twieg, and B. D. Dunietz "Enhancing charge mobilities in selectively fluorinated oligophenyl organic semiconductors: a design approach based on experimental and computational perspectives" *J. Mater. Chem. C.*, **7** (2019) 3881-3888.

38. S. Bhandari, M. Cheung, E. Geva, L. Kronik, and B. D. Dunietz "Fundamental Gaps of Condensed-Phase Organic Semiconductors from Single-Molecule Calculations using Polarization-Consistent Optimally Tuned Screened Range-Separated Hybrid Functionals" *J. Chem. Theory Comput.*, **14** (2018) 6287-6294.

39. S. Sarkar, J. D. Protasiewicz, and B. D. Dunietz "Controlling the Emissive Activity in Heterocyclic Systems Bearing C=P Bonds" *J. Phys. Chem. Lett.*, **9** (2018) 3567-72.

40. X. Sun, P. Zhang, Y. Lai†, K. L. Williams, M. S. Cheung, B. D. Dunietz, and E. Geva "Computational Study of Charge-Transfer Dynamics in the Carotenoid–Porphyrin–C60 Molecular Triad Solvated in Explicit Tetrahydrofuran and Its Spectroscopic Signature" *J. Phys. Chem. C.*, **122** (2018) 11288-99.

41. 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.

42. 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.

43. 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.

44. 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.

45. 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.

46. 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.

47. 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.

48. 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.

49. 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.

50. 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.

51. 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.

52. 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.

53. 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.

54. 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.

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

56. 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.

57. 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.

58. 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.

59. 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.

60. 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.

61. 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.

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

63. 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.

64. 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.

65. 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.

66. 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.

67. 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.

68. 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.

69. 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.

70. 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.

71. 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.

72. 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.

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

74. 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.

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

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

77. 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.

78. 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.

79. 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.

80. 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.

81. 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.

82. 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.

83. 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.

84. 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.

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

86. 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.

87. 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.

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

89. 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.

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

91. 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.

92. 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.

93. 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.

94. 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.

95. 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.

96. 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.

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

98. 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.

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100. 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.

101. 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.

102. 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.

103. 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.

104. 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.

105. 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.

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

107. 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.

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

109. 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.

110. 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.

111. 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
  - TSRC workshop: Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy. "Dielectric Screened Range Separated Hybrid Functionals - A Polarization Consistent Framework for Describing Photoinduced Electron Transfer and Transport Processes" Telluride, CO (October 2023)
  - Electronic Transport in Molecular Quantum Conductors, "Predictive modeling of electron transport based on modern density functional theory", Rehovot, Israel (June 2023)
  - Non-Equilibrium dynamics of Condensed Matter, "Mapping out electronic energy and charge transfer pathways in the tetraphenyldibenzoperiflanthene/fullerene interfacial dimer" Yearim Hotel, Ma'ale Hahamisha, Israel (April 2023)
  - ACS Spring 2023 symposium on QM/QM and embedding models "Dielectric Screened Range Separated Hybrid Functionals - A Polarization Consistent Framework for Describing Photoinduced Electron Transfer and Transport Processes", Indianapolis, IN (March 2023)
  - EMSL integration 2022 "Modeling Photo Induced Electron transfer and transport in Natural Photosystems. An ab-initio perspective on kinetics", Richland, WA (Oct. 2022)
  - 2021 Computational and Theoretical Chemistry PI Meeting "Predictive descriptions of photoinduced processes usin g a comprehensive multiscaling computational framework based and linearized semiclassical rate theory and environment polarization consistent electronic structure" DOE Workshop (Aug. 2021)
  - TSRC workshop: Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy "Predictive description of photo or bias-induced electron transfer or transport processes through molecular-resolved interfaces using an environment polarization consistent framework" Telluride, CO (July 2021)

- AMLCI Materials Day 2021 "Modeling Photo and Bias Induced Electron transfer and transport. An ab-initio perspective on kinetics" (April 2021)
- Adim Physics Days VIII, "Modeling Photo and Bias Induced Electron transfer and transport. An ab-initio perspective on kinetics" Bilecik, Turkey (Sept. 2019)
- TSRC workshop: Non-equilibrium Phenomena, Nonadiabatic Dynamics and Spectroscopy "Molecular and dielectric impact on the spectra, energy and charge transfer processes in interfaces of organic semiconducting materials: A predictive comprehensive computational framework", Telluride, CO (July 2019)
- American Chemical Society "Predictive description of photo-induced electron transfer or transport through molecular-resolved interfaces", Boston, MA (Aug. 2018)
- 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 2007)
  - Lester Fest Symposium, Berkeley, CA (March 2007)

- Contributed Lectures in Scientific Meetings

  - ACS Goddard fest; Boston, MA (August 2007)
  - APS " Transport through nanostructures" session; Denver, CO (March 2007)
  - ACS special "hydrogen storage material" session; San Francisco, CA (Sept. 2006)
  - TDDFT Workshop; Benasque, Spain August 2006 (presented a poster)
  - ACS "Molecular electronics" session; Atlanta, GA (March 2006)
  - American Computational and Theoretical Chemistry (ACTC); UCLA, CA (July 2005); (presented two posters)

- Conference Chair and Organizer

  - American Physical Society; Boston MA (March 2012) Session chair: "Focus Session: DFT V: Partitioning and Embedding Theories; Finite-Temperature".
  - Gordon research conference on time dependent density functional theory, Biddeford, ME (August 2011), session chair.
  - American Computational and Theoretical Chemistry (ACTC); Northwestern University, Chicago, IL (July 2008) Session chair.
  - 40th Midwest Theoretical Chemistry Conference (June 2008). Co-organizer with Prof. E. Geva.
  - APS - "Transport through nanostructures" session; Denver, CO (March 2007). Co-organizing with Prof. Hongkun Park.

- Departmental seminars

  - Kent State University, Chemistry (November 2022)
  - University of Oklahoma, Chemistry (November 2022)
  - University of Delaware, Chemistry (September 2022)
  - Bar-Ilan University, Chemistry (June 2022)
  - Hebrew University in Jerusalem, Chemistry (June 2022)
  - Weizmann Insitute, Chemistry (May 2022)
  - Ohio State University, Chemistry (October 2021)
  - Akron University, Chemistry (February 2021)
  - Youngstown State University, Chemistry, Youngstown, OH (February 2017)
  - Kent State University, Chemistry, Kent, OH (February 2015)
  - Los Alamos National laboratory, NM (May 2014)
  - Wright State University, OH (December 2013)
  - Weizmann Institute of Science, Materials Science and Physical Chemistry departments, Tel-Aviv, Israel (July 2013)
  - Houston University, Physics, Houston, TX (April 2013)
  - Liquid crystal institute, Kent state university, Kent, OH (March 2013)
  - Wayne state university, Detroit, MI (April 2012)
  - Oakland university, MI (April 2012)
  - Kent State university, Kent, OH (March 2012)
  - Pacific Northwest National Laboratory (March 2012)
  - University of Maryand, Baltimore County, Physics department (March 2012)
  - Rutgers University, Newark, NJ (December 2011)
  - Michigan State University, MI (March 2011)
  - University of Northern Texas, TX (February 2011)
  - Bowling Green State University, OH (December 2010)
  - Bar-Ilan University, Ramat-Gan, Israel (November 2009)
  - The Technion, Haifa, Israel (November 2009)

- Tel-Aviv University, Tel-Aviv, Israel (November 2009)
- Ben-Gurion University, Beer-Sheva, Israel (November 2009)
- Columbia University (November 2009)
- Boston University; Greater Boston theoretical chemistry seminars (October 2009)
- Harvard Uni; Greater Boston theoretical chemistry seminars (October 2009)
- M.I.T, Cambridge; Greater Boston theoretical chemistry seminars (October 2009)
- University of Washington, Seattle (May 2009)
- Georgia Tech (May 2009)
- University of Wisconsin at Madison; Material engineering seminars (March 2009)
- University of Southern California (February 2009)
- University California at LA (February 2009)
- University California at Irvine (February 2009)
- Indiana University at Bloomington (January 2009)
- Notredam university (January 2009)
- Ohio State (November 2008)
- Hebrew University, Jerusalem, Israel (October 2008)
- Wayne State University (October 2008)
- University of Arizona (Sept. 2008)
- University of Georgia (August 2008)
- University of Florida at Gainsville (April 2008)
- University of Wisconsin at Madison (March 2008)
- Rochester University (March 2008)
- Cornell University (March 08)
- Northwestern University (January 2008)
- Michigan State University (Sept. 2007)
- Central Michigan University (December 2006)
- Western Michigan University (November 2006)
- Oakland University (2005)

Research Group Members

- Current Postdoctoral Fellows

  Erkan Kose

- Current Graduate Students (Research Assistants)

  Roshan Khatri
  Aswathy Jayachandran
  Abhishek Bagale

Slater Bakenhaster

- Current Undergraduate Students

  Eli Holder

- Former Postdoctoral Fellows

  Dr. Max Saller (2022-2024)
  Dr. Chandrima Chakarvartry (2020-2022)
  Dr. Bikash Mandal (2020-2022)
  Dr. Huseyin Aksu (2018-2020)
  Dr. Ariela Kaspi (2018-2019)
  Dr. Buddhadev Maiti (2014-2015, 2018-2019)
  Dr. Alex Schubert (2016-2018 ICAM fellow, was co-mentored with Prof. Geva [UM])
  Dr. Sunandan Sarkar (2016-2017)
  Dr. Atsushi Yamada (2015-2017)
  Dr. Qingguo Feng (2014-2015)
  Dr. Arun K Manna (2013-2014)
  Dr. Myeong Lee (2012-2014)
  Dr. Zilong Zheng (2013-2014)
  Dr. Parta Pal (2011-2012)
  Dr. Shauhui Zheng (2010-2012)
  Dr. Nikolai Sergueev (2010-2011)
  Dr. Trilisa Perrine (2005-2008)
  Dr. Zhen Zhao (2007)
  Dr. Mousumi Das (2005-2006)
  Dr. Corneliu Buda (2004-2006)
  Dr. Yunqing Chen (2004-2005)

- Former Graduate Students

  Dr. Khadiza Begam (Physics, KSU 06/2023)
  Dr. Srijana Bhandari (Chemistry, KSU 09/2020)
  Dr. Heidi Phillips (Chemistry, UM, 04/2015)
  Dr. Alexander Prociuk (Physics, UM, 08/2009)

- Rotation (visiting) Graduate Students

Mr. Bishnu Pant	Ms. Jessica Donheue
Ms. Bei Ding	Ms. Surma Talapatra
Mr. Sung Hei	Mr. Tim Berto
Mr. Carlos Baiz	Mr. Brannon Gary
Mr. Ron Smith	Ms. Miri Shlomi

- Former Undergraduate and High School (HS) Research Students

Mr. John Stewart (2022 REU)	Mr. Eli Holder (2021-2022)
Mr. Sawyer Huckbee (2020-22, HS)	Mr. Jameson Payne (2019, HS)
Mr. Austin Hoskins (2017, HS)	Mr. Kevin Fenk (2015, HS)
	Ms. Jessica Shost
Mr. Jacob Smith	Ms. Vicotria Washington
Ms. Francis Devine	Mr. Alexander Hyla
Mr. Robert Liu	Mr. Tatsuya Kamiya
Ms. Sarah Ledford	Mr. Miguel Wong
Mr. Ben Van Kuiken	Mr. Christopher Lee Marsh

Service

- Departmental Service

  Graduate Studies Coordinator (2024)

  Graduate Studies, assisting the graduate studies coordinator to overhaul of the graduate studies curriculum (2021-22)

  Graduate Studies and Admission Committee, member (2012-2017, 2021-2022)

  Undergraduate Student Grievance, chair (2019-2021)

  Student Celebration Award Ceremony, chair (2020-2021)

  Academic Advisor, minor in chemistry (2020-2021)

  Physical Chemistry, division chair (2017-2022)

  Curriculum Committee, member (2017-2021)

  Faculty Search Committees Analytical and Physical Chemistry

  Recruitment Committee

  High School Student Research Mentor

- University Service

  Admission Committee, Material Science Graduate Program, member (2021-22)

  Material Science Graduate Program, Seminar Chair (2021-22)

  Reviewer of university seed projects

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

- Graduate Student Dissertation Committees

  Ryan Williams (MSGP, candidacy, 2022)

  Ruilin Xiao (MSGP, defense, 2022)

  Abdulaziz Alqahtani (Math., defense, 2022)

  Ugochukwu Ugwu (Mathematics, defense, 2021)

  Matthew Deutch (AMLCI, candidacy, 2021)

  Babak Salehi Kasmaei (Mathematics, defense, 2021)

Corrine Callison (AMLCI, candidacy, 2020)

Srijana Bhandari (Chemistry, chair, 2018)

Sajedeh Afghah (LCI, defense, 2018)

Heidi Phillips (Chemistry, chair, 2016)

Randall Breckon (Chemistry, candidacy 2012)

Alexander Prociuk (Chemistry, chair, 2010)

- Wide research community Service

  Ohio Transfer 36 faculty review panel, Natural Sciences Member. Ohio Articulation & Transfer Network, Ohio Department of Higher Education (2023-2024)

  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 2008)

  Co-organizing with Prof. Hongkun Park from Harvard University a focus session on "Electron Transport in Nanostructures" in the APS national March 2007 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)