

Barry D. Dunietz

Curriculum Vitae

(as of December, 2011)

Work Address

Department of Chemistry
University of Michigan
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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

- 2004–Present **Assistant Professor of Chemistry**
Department of Chemistry, University of Michigan, Ann Arbor.
- 2001–2004 **Post Doctoral research scientist** with *Prof. M. Head-Gordon*
Department of Chemistry, University of California, Berkeley.
- 1995–2000 **Graduate student and research assistant** with *Prof. R. Friesner*
Department of Chemistry, Columbia University, New York.
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 – University of Michigan

- 2004 Quantum Chemistry (Chem 571)
2005-2006,2008 Computational Chemistry Laboratory (Chem 462)
2007 Physical Chemistry I (Chem 461)
2007-2010 General Chemistry: Macroscopic Investigations
and Reaction Principles (Chem 130)
2010-2011 Chemical Principles and Introduction to quantum chemistry (Chem 260/261)

Currently Funded Research Grants

1. Single PI: “Electronic-structure modeling of electron transport switching in energy conversion schemes”, funded by DOE-BES (2010-2013, \$406,000).
2. Co-PI: “Center for solar and thermal energy conversion in complex materials (CSTECCM)” (PI: P. Green); a DOE-Energy Frontier Research Center (EFRC) (08/01/09 - 07/31/14; \$19,500,000 for Center; \$517,582 to Dunietz laboratory).

Publications

1. Balachandran, R. and Reddy, P. and Dunietz, B. D. and Gavini, V., “End group induced charge transfer in molecular junctions: Effect on thermopower”, **Pending final revisions** (2011).
2. Ryota, K. and Perez-Bolivar, C. and Smith, J. and Dunietz, B. D. and Anzenbacher Jr., P., “Dibenzophosphole Chalcogenides: Synthesis and Modeling of Structure and Optical Properties”, **Pending final revisions** (2011).
3. Meoyong, L. and Pramod, R. and Dunietz, B. D., “Active Control of Thermal Transport in Molecular Junctions with Ferromagnetic Electrodes”, **Pending final revisions** (2011).
4. Zheng, S. and Phillips, H. and Geva, E. and Dunietz, B. D., “*Ab-initio* study of the emissive charge-transfer states of solvated chromophore-functionalized silsesquioxanes”, **Submitted** (2011).
5. Phillips, H. and Zheng, S. and Hyla, A. and Laine, R. and Goodson III, T. and Geva, E. and Dunietz, B. D., “*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.*, **Accepted** (2011).
6. Tan, A. and Sadat, S. Balchandran, J. and Gavini, V. and Dunietz, B. D. and Jang, S.-Y. and Reddy, P., “Effect of Length and Contact Chemistry on the Electronic Structure and Thermoelectric Properties of Molecular Junctions”, *J. Amer. Chem. Soc.*, **132** (2011), 2914-18.
7. Sergueev, N. and Seungha S. and Kaviany, M. and Dunietz, B. D., “Efficiency of thermoelectric energy conversion in biphenyl-dithiol junction: the effect of electron-phonon interaction”, *Phys. Rev. B.*, **83**, , (2011), 195415.
8. Philips, H. and Prociuk, A. and Dunietz, B. D., “Bias effects on the electronic spectrum of a molecular bridge”, *J. Chem. Phys.*, **134** (2011), 54708.
9. Ding, B. and Washington V. and Dunietz, B. D., “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.
10. Prociuk, A. and Dunietz, B. D., “Photo-induced absolute negative current in a molecular electronic system.” *Phys. Rev. B.*, **82**, (2010), 125449.
11. Prociuk, A. and Phillips, H. and Dunietz, B. D., “Modeling transient aspects of coherence-driven electron transport”, *J. Phys.: Conf. Ser.* **220**, (2010), 012008.

12. Perrine, T. and Dunietz, B. D.; "Contact geometry symmetry dependence of field effect gating in single molecule transistors", *J. Amer. Chem. Soc.*, **132**, (2010), 2914.
13. Baiz, C. and Ledford, S. J. and Kubarych, K and Dunietz, B. D., "Intermolecular Double Hydrogen-atom Transfer Reactions", *J. Phys. Chem. A.*, **113**, (2009), 4862.
14. Prociuk, A. and Dunietz, B. D., "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.
15. Wong, M. and Van-Kuiken, B and Buda, C. and Dunietz, B. D., "Multi adsorption and Coadsorption of Hydrogen on model conjugated systems" , *J. Phys. Chem. C.*, **113**, (2009), 12571.
16. Perrine, T. M. and Berto, T. and Dunietz, B. D., "Enhanced Conductance via Induced π -Stacking Interactions in Cobalt(II) Terpyridine Bridged Complexes", *J. Phys. Chem. B.* **112** (2008), 16070.
17. Perrine, T. and Dunietz, B. D., "Conductance of a cobalt(II) terpyridine complex based molecular transistor: A computational analysis", *J. Phys. Chem. A.*, **112**, (2008), 2043.
18. Geyer, A. M., Wiedner, E. S., Gary, J. B., Gdula, R. L., Kuhlmann, N. C., Johnson, M. J. A., Dunietz, B. D. and Kampf J. W., "Synthetic, mechanistic, and computational investigations of nitrile-alkyne cross-metathesis", *J. Amer. Chem. Soc.*, **130**, (2008), 8994-8999.
19. Gary, J. B., Buda, C., Johnson, M. J. A. and Dunietz, B. D., "Accessing metal-carbide chemistry - A computational analysis", *Organometallics*, **27**, (2008), 814-826.
20. Zhao, Z. and Dunietz B. D., "Ab initio study of charge transport of hydrogen functionalized palladium wires", *J. Chem. Phys.*, **129**, (2008), 024702.
21. Perrine, T. M. and Smith, R. G. and Marsh, C. and Dunietz, B. D., "Gating of single molecule transistors: Combining field-effect and chemical control", *J. Chem. Phys.*, **128**, (2008), 154706.
22. Prociuk, A. and Dunietz, B. D., "Time-dependent current through electronic channel models using a mixed time-frequency solution of the equations of motion", *Phys. Rev. B.*, **78**, (2008), 165112.
23. Das, M. and Dunietz, B. D., "Electron Transport through Heterogenous Intermolecular Tunnel Junctions", *J. Phys. Chem. C.*, **111**, (2007), 1535-1540.
24. Perrine, T. and Dunietz, B. D., "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.
25. Perrine, T. and Dunietz, B. D., "Carbonyl mediated conductance through metal bound peptides; a computational study", *Nanotechnol.*, **18** (2007), 424003.
26. Baiz, C. R. and Dunietz, B. D., "Theoretical studies of conjugation effects on excited state intramolecular hydrogen-atom transfer reactions in model systems", *J. Phys. Chem. A.*, **111**, (2007), 10139-10143.

27. Kendler, S., Lambertus, G. R., Dunietz, B. D., Coy, S. L., Nazarov, E. G., Miller, R. A. and Sacks, R. D., "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.
28. Prociuk, A. and Dunietz, B. D., "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.
29. Chen, Y., Prociuk, A., Perrine, T. and Dunietz, B. D., "Spin-dependent electronic transport through a porphyrin ring ligating an Fe(II) atom: An ab initio study", *Phys. Rev. B.*, **74**, (2006), 245320-9.
30. Buda, C., Caskey, S. R., Johnson, M. J. A. and Dunietz, B. D., "Metathesis-enabled formation of a terminal Ru Carbide complex: A computational study", *Organometallics*, **25**, (2006), 4756-4762.
31. Buda, C. and Dunietz, B. D., "Hydrogen Physisorption on the Organic Linker in Metal Organic Frameworks: Ab Initio Computational Study", *J. Phys. Chem B.*, **110**, (2006), 10479.
32. Yihan Shao *et al.*, "Advances in methods and algorithms in a modern quantum chemistry program package" *Phys. Chem. Chem. Phys.* **8** (2006), 3172.
33. Dunietz, B. D. and Markovic, N. and Ross, P. H. and Head-Gordon, M., "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.
34. Ugalde, J. M. and Dunietz, B. D. and Dreuw, A. and Head-Gordon, M. and Boyd, R. J., "The spin dependence of spatial size of Fe(II) and of the structure of Fe(II)-porphyrins", *J. Phys. Chem A.*, **108**, (2004), 4653.
35. Head-Gordon, M. and Van Voorhis, T. and Beran, G. J. O. and Dunietz, B. D., "Local correlation models", (Chapter Book) *Computational Science - ICCS* **2660** (2003), 96.
36. Saravanan, C. and Dunietz, B. D. and Markovic, N. and Somorjai, G. and Head-Gordon, M. Ross, P. H. "Electro-oxidation of CO on Pt electrodes simulated by electronic structure calculations" *J. Electroanal. Chem.* **554**, (2003), 459.
37. Dunietz, B. D. and Head-Gordon, M., "Manifestations of symmetry breaking in self-consistent field electronic structure calculations" *J. Phys. Chem A.*, **107**, (2003), 9160.
38. Dunietz, B. D. and Dreuw, A. and Head-Gordon, M., "Initial steps of the photodissociation of the CO ligated heme group", *J. Phys. Chem B.*, **107**, (2003), 5623.
39. Dunietz, B. D. and van Voorhis, T. and Head-Gordon, M., "Geometric direct minimization of Hartree Fock calculations involving open shell wavefunctions with spin restricted orbitals", *J. Theo. Comp. Chem.*, **1**, (2002), 255.
40. Dreuw, A. and Dunietz, B. D. and Head-Gordon, M., "Characterization of the relevant excited states in the photodissociation of the CO-ligated Hemoglobin and Myoglobin", *J. Amer Chem. Soc.*, **124**, (2001), 12070.

41. Dunietz, B. D. and Friesner, R. A., "Application and development of multiconfigurational localized perturbation theory", *J. Chem. Phys.* **115**, (2001), 11052.
42. Gherman, B. F. and Dunietz, B. D. and Whittington, D. A. and Lippard, S. J. and Friesner, R. A., "Activation of the C-H bond of methane by intermediate Q of methane monooxygenase: A theoretical study", *J. Amer Chem. Soc* **123**, (2001), 3836.
43. Friesner, R. A. and Dunietz, B. D., "Large-scale ab-initio quantum chemical calculations on biological systems", *Acc. Chem. Res.* **34**, (2001), 351.
44. Dunietz, B. D. and Beachy, M. D. and Cao, Y. X. and Whittington, D. A. and Lippard, S. J. and Friesner, R. A., "Large scale ab-initio quantum chemical calculation of the intermediate in the soluble methane monooxygenase catalytic cycle", *J. Amer Chem. Soc*, **122**, (2000), 2828.
45. Friesner, R. A. and Murphy, R. B. and Beachy, M. D. and Ringnalda M. N. and Pollard, W. T. and Dunietz, B. D. and Cao, Y. X., "Correlated ab-initio electronic structure calculations for large molecules", *J. Phys. Chem. A.*, **103**, (1999), 1913.
46. Dunietz, B. D. and Murphy, R. B. and Friesner, R. A., "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
 - Gordon research conference on time dependent density functional theory(invited session chair and speaker), Biddeford, Maine (August 11)
 - Workshop on computational molecular electronics; Telluride, Co. (August 11)
 - Workshop on Simulation and Modeling of Emerging Electronics; Hong-Kong, China (Dec. 10)
 - An International Conference in Honor of Professor Henry F. Schaefer III; Berkeley, Ca. (May 10)
 - Workshop on "Theoretical, Computational, and Experimental Challenges to Exploring Coherent Quantum Dynamics in Complex Many-Body Systems"; Dublin, Ireland; (May 10)
 - Also participated in the workshop: "Quantum transport and dynamics in materials and biosystems: From molecular mechanisms to mesoscopic functionality"; Dublin, Ireland; (May 10)
 - NSF workshop on progress in physical organic chemistry; Austin, Tx. (January 10)
 - "Progress in Non-Equilibrium Green's Function (PNEGF) workshop"; Glasgow, Scotland (August 09)
 - Workshop on computational molecular electronics; Telluride, Co. (July 09)
 - APS: Focus session on computational molecular electronics (March 09)
 - International Society for Theoretical Chemical Physics (ISTCP)-VI; Vancouver (July 08)

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- Thirteenth International Workshop on quantum systems in chemistry and physics QSCP-XIII; Lansing, Mi. (July 08)
 - The Gentner-Minarva Time-Dependent Density-Functional-Theory symposium; Eilat, Israel (December 07)
 - Lester Fest Symposium; Berkeley, Ca. (March 07)
 - 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. (September 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 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).
 - Invitations Declined
 - WUN-SPintronics 2010 and the Materials Computation Summer School, University of Illinois (June 10).
 - Departmental seminars
 - Michigan State University, MI. (March 11)
 - University of Northern Texas, TX. (February 11)
 - University of Toledo, OH. (December 10)
 - 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 seminar series (October 09)
 - Harvard, Cambridge ; Greater Boston Theoretical chemistry seminar series (October 09)

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- M.I.T, Cambridge; Greater Boston Theoretical chemistry seminar series (October 09)
 - University of Washington, Seattle (May 09)
 - Georgia Tech (May 09)
 - University of Wisconsin at Madison (Material engineering seminar series) (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 (September 08)
 - University of Georgia (August 08)
 - University of Florida at Gainesville (April 08)
 - University of Wisconsin at Madison (March 08)
 - Rochester University (March 08)
 - Cornell University (March 08)
 - Northwestern University (January 08)
 - Michigan State University (September 07)
 - Central Michigan University (December 06)
 - Western Michigan University (November 06)
 - Oakland University (05)

Research Group Members

- Current Postdoctoral Fellows

Dr. Shaohui Zheng

Dr. Partha Pal

Dr. Myeong Lee

- Current Graduate Students (Research Assistants)

Ms. Heidi Phillips

Mr. Janakiraman Balachandran (Ram), Dept. of Mech. Eng. (mentored by Prof. Vikram Gavini)

- Current Undergraduate Students

Ms. Victoria Washington

Mr. Pavel Okun

Ms. Jessica Shost

- Former Postdoctoral Fellows

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. Alexander Prociuk: Physics Graduate Student (01/05-08/09)

- 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. Jacob Smith

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

- 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 Laboratory (NETL).
 - Israel Science Foundation (ISF).
 - National Science Foundation (NSF)
 - Petroleum Research Fund (PRF)
- University Service
 - Refereed proposals for university seed projects (Graham institute)
 - Served on several students committees (physics, applied physics and engineering programs).
- Departmental Service
 - Physical Chemistry seminar coordinator
 - Physical Chemistry candidacy seminar coordinator
 - Gomberg Lecture committee
 - Admissions Committee
 - Recruiting Committee
- Graduate Student Dissertation Committees
 - Brannon Gary (Chemistry, Sanford)
 - Changgua Zhen (Material Science and Engineering, Kieffer)
 - Carlos Baiz (Chemistry, Kubarych)
 - Michael Orozco (Chemistry, Sension)
 - Frank Vazquez (Chemistry, Geva)
 - Henry Boateng (Mathematics, Krasny)
 - William Fisher (Applied Physics, Rand)
 - Meng Guo (Chemistry, Goodson)
 - John Hensslor (Chemistry, Matzger)
 - Damian Khan (Applied Physics, Orr).
 - Yunqing Chen (Physics, Banaszak Holl and Orr)
 - Chenyue Xing (Chemistry, Andricioaei)