
Barry D. Dunietz

Short Curriculum Vitae (as of Aug., 2016)

Full CV is available upon request

Work Address

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Academic positions and education

- 2016–Present **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.
- 1995–2000 **Graduate student and research assistant** with *Prof. R. Friesner*
Department of Chemistry, Columbia University, New York.
- 1994–1995 **Research assistant** with *Prof. U. Kaldor*
Chemistry Department, Tel-Aviv university, Israel.
- 1994 **B.Sc.** Chemistry major & Computer Science minor; Magna cum Laude
Chemistry Department, Tel-Aviv University, Israel

Recent Funded Research Grants

1. Co-PI (Lead): “ Post-Marcus theory and simulation of interfacial charge transfer dynamics in organic semiconducting materials” PIs: Cheung (University of Houston), Dunietz (Kent State University), Geva (University of Michigan) Source of support: DOE-BES (2016-2017, \$996,000).
2. Single PI: “Charge transfer, injection and mobility in organic semi-conducting materials: modeling for insight on mechanistic aspects”. Source of support: NSF (2014-2017, \$325,683).
3. Co-PI (lead): ”Ab-initio molecular modeling of electron transfer and transport in organic semiconductor crystals. Source of support: Institute for Complex Adaptive Matter” (2014-2016, \$50,000).
4. Single PI: “Electronic-structure modeling of electron transport switching in energy conversion schemes Source of Support: Department of Energy, Basic Energy Sciences”. Source of support: DOE-BES (2010-2016, \$406,000).

Selected Recent Publications

The following is representative list of recent publications from over sixty (60) peer reviewed publications. (full list is attached separately):

- Yamada, A. and Feng, Q. and Hoskins, A. and Fenk, K. and Dunietz, B. D., “Achieving Predictive Description of Molecular Conductance by using a Range-Separated Hybrid Functional” , *Nano. Lett.*, **Accepted** (2016).
- Feng, Q. and Atsushi, Y. and Baer, R. and Dunietz, B. D., “Deleterious effects of exact exchange functionals on predictions of molecular conductance” *J. Chem. Theory Comput.*, **12** (2016) 3431-3435.
- Manna, A. K. and Balamurugan, D. and Cheung, M. S. and Dunietz, B. D., “Unraveling the Mechanism of Photoinduced Charge Transfer in Carotenoid-Porphyrin-C₆₀ Molecular Triad”, *J. Phys. Chem. Lett.*, **6** (2015) 1231-1237.
- Wilcox, D. E. and Lee, M. H. and Sykes, M. E. and Niedringhaus, A. and Geva, E. and Dunietz, B. D. and Shtein, M. and Ogilvie, J. P. “Ultrafast Charge-Transfer Dynamics at the Boron Subphthalocyanine Chloride/C60 Heterojunction: Comparison Between Experiment and Theory” *J. Phys. Chem. Lett.*, **6** (2015) 569575.
- Zilong, Z. and Manna, K. M. and Phillips, H. and Hammer, M. and Song, C. and Geva, E. and Dunietz, B. D., “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.
- Lee, M. H. and Dunietz, B. D. and Geva, E., “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.
- Manna, K. M. and Dunietz, B. D., “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.
- Phillips, H. and Zheng, Z. and Geva, E. and Dunietz, B. D., “Orbital Gap Predictions for Rational Design of Organic Photovoltaic Materials”, *Opto Elect.*, **15** (2014) 1509-1520.
- Lee, M. H. and Dunietz, B. D. and Geva, E., “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) 9780-9789.
- Lee, M. H. and Dunietz, B. D. and Geva, E., “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