

Barry D. Dunietz

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GENERAL INFORMATION:

- Born: November 12, 1968, New-York, NY. Married +3.
- **1987-90** - Military Service (IDF).

EDUCATION:

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

RESEARCH EXPERIENCE

- Since **Fall 2004**: Assistant Prof. at the University of Michigan at Ann Arbor, Department of Chemistry.
 - Molecular conductance systems:
 1. Spin dependent transmission (iron-porphyrin devices).
 2. Chemical sensors (transmission in tunnel junctions and related orientation effects).
 3. Conjugated organic molecule as field effect transistors (geometry/orientation effects).
 - Method development for molecular transport:
 1. Strong coupling extension of the Landauer scheme.
 2. Time Dependent DFT implementation of NEGF.
 3. TDDFT of extended systems.
 - Hydrogen fuel economy:
 1. Hydrogen physisorption on conjugated systems.
 2. Hydrogen generating reactions.
 - Metal catalyzed reaction mechanism:
 1. Ru-carbide formation from metathesis reaction.
 - Electronic spectra of systems with biological relevance (Cobalamine).
- **2001-2004** Post Doctoral research scientist with *Prof. M. Head-Gordon*, University of California at Berkeley.

- New coupled cluster methodology for open shell systems.
- Quantum chemistry investigation of complex systems.
- **1995-2000** Graduate student, Columbia University, New York, N.Y Work with *Prof. R. Friesner*. Thesis Topics:
 - Development and application of multi configurational localized perturbation theory.
 - Biological applications of quantum chemistry methodologies.
- **1994-1995** Research assistant with *Prof. U. Kaldor*, Chemistry Department, Tel-Aviv university.

PUBLICATION LIST

References

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- [2] Zhao, Z. and D., Dunietz B. ‘Ab initio study of charge transport of hydrogen functionalized palladium wires.’ *J. Chem. Phys.*, **129**, (2008), 024702.
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- [6] 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.
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- [9] 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.
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