

Rigoberto Hernandez  
Department of Chemistry  
Remsen Hall  
Johns Hopkins University  
Baltimore, MD 21218

Biographical Sketch, August 23, 2018  
410.516.4018, phone  
410.516.8024, fax  
[r.hernandez@jhu.edu](mailto:r.hernandez@jhu.edu)  
[rh.jhu.edu/web](http://rh.jhu.edu/web)

#### A. Professional Preparation

Princeton University (Princeton, NJ)	Chem. Engr. & Math.	B.S.E. ( <i>high honors</i> )	1989
University of California (Berkeley, CA)	Chemistry	Ph.D.	1993
Weizmann Institute (Rehovot, ISRAEL)	Chemical Physics	postdoctoral	1994
University of Pennsylvania (Philadelphia, PA)	Chemistry	postdoctoral	1995-96

#### B. Appointments

2016-present	Gompf Family Professor of Chemistry, Johns Hopkins University
2012-present	Director, Open Chemistry Collaborative in Diversity Equity (OXIDE)
2016-2018	Adjunct Professor of Chemistry, Georgia Institute of Technology
2009-2016	Professor of Chemistry, Georgia Institute of Technology
2000-2016	Co-Director, Center for Computational Molecular Science & Technology
2002-2009	Associate Professor of Chemistry, Georgia Institute of Technology
1996-2002	Assistant Professor of Chemistry, Georgia Institute of Technology

#### C. Honors and Awards

Herty Medal (2017); Transformative Research and Exceptional Education (TREE) Award, Research Corporation (2016); Visiting Scholar, Phi Beta Kappa Society (2015-2016); Diversity Award, Council for Chemical Research (2015); **ACS Award** for Encouraging Disadvantaged Students into Careers in the Chemical Sciences (2014); **APS Fellow**, American Physical Society (elected 2011); Vasser Woolley Faculty Fellow (2011-2013); **ACS Fellow**, American Chemical Society (elected 2010); Sackler Visiting Chair in Exact Sciences, Tel Aviv University (2010); Alexander von **Humboldt Research Fellow** (2006); **AAAS Fellow**, American Association for the Advancement of Science (elected 2004); Goizueta Foundation Junior Rotating Faculty Chair (2002-2006); BPP Freshman Partner of the Year Award (Georgia Tech, 2002); Sigma Xi Southeast Regional Young Investigator (2000 & 2002); Blanchard Assistant Professor of Chemistry (1999-2001); **Sloan Fellow**, Alfred P. Sloan Foundation (2000-2003); **Cottrell Scholar**, Research Corporation (1999-2004); NSF CAREER Award (1997-2002); Sigma Xi Young Faculty Award (Georgia Tech, 1999); Feinberg Postdoctoral Fellowship (1994), NSF Graduate Research Fellowship (1989-1993), AT&T Cooperative Research Fellowship (1989-1993)

#### D. Products (12 selected out of over 115 peer-reviewed articles and 6 editorials)

1. R. Hernandez, D. Stallings and S. K. Iyer (Eds.), ACS Symposium Series 1277, (American Chemical Society, Washington DC, 2018). Peer reviewed book. ([doi:10.1021/bk-2018-1277](https://doi.org/10.1021/bk-2018-1277))
2. Q. Cui, R. Hernandez, S. E. Mason, T. Frauenheim, J. A. Pedersen, and F. Geiger, "Mini-review. Sustainable Nanotechnology: Opportunities and Challenges for Theoretical/Computational Studies," *J. Phys. Chem. B* **120**, 7297-7306 (2016).
3. H. R. Bureau, E. Hershkovits, S. Quirk and R. Hernandez, "Determining the energetics of small  $\beta$ -sheet peptides using Adaptive Steered Molecular Dynamics," *J. Chem. Theory Comput* **12**, 2028 (2016).
4. G. T. Craven and R. Hernandez, "Lagrangian descriptors of thermalized transition states on time-varying energy surfaces," *Phys. Rev. Lett.* **115**, 148301 (2015).
5. C. Murphy, A. Vartanian, F. Geiger, R. Hamers, J. Pedersen, Q. Cui, C. Haynes, E. Carlson, R. Hernandez, R. Klaper, G. Orr, Z. Rosenzweig, *ACS Central Science* **1**, 117 (2015).
6. "Communication: Transition state trajectory stability determines barrier crossing rates in chemical reactions induced by time-dependent oscillating fields," G. T. Craven, T. Bartsch and R. Hernandez, *J. Chem. Phys.* **141**, 041106 (2014). (*Communication*)

7. G. Ozer, S. Quirk and R. Hernandez, "The thermodynamics of decaalanine stretching in water obtained by adaptive steered molecular dynamics simulations," *J. Chem. Theory Comput.* **8**, 4837-4844 (2012).
8. "Dynamical Simulation of Dipolar Janus Colloids: Equilibrium Structure and Thermodynamics," M. Hagy and R. Hernandez, *J. Chem. Phys.* **137**, 044505 (2012).
9. "The ontology of temperature in nonequilibrium systems," A. V. Popov, R. Hernandez, *J. Chem. Phys.* **126**, 244506:1-16 (2007).
10. "Dynamics of swelling/contracting hard spheres surmised by an irreversible Langevin equation," A. V. Popov, J. Melvin, and R. Hernandez, *J. Phys. Chem. A* **110**, 1635-1644 (2006).
11. "Probing the Cybotactic Region in Gas-Expanded Liquids (GXLs)," J. P. Hallett, C. L. Kitchens, R. Hernandez, C. L. Liotta, and C. A. Eckert, *Acc. Chem. Res.*, **39**, 531-539 (2006).
12. "The mechanism for radical cation transport in duplex DNA oligonucleotides," C.-S. Liu, R. Hernandez, and G. B. Schuster, *J. Am. Chem. Soc.* **126**, 2877-2884 (2004).

#### E. Synergistic Activities (representative activities)

1. **Professional Service:** District IV Director, Board of Directors, American Chemical Society (2014-2019); heavily involved in national ACS Governance activities since 2003.
2. **Education:** Chair/Founder, Academic Leadership Training (ALT) Workshop (2016,2017), Co-Instructor/Founder, NSF-supported cCWCS workshop on Theoretical and Computational Chemistry targeted at undergraduate college professors (2002-05, 2009, 2011, 2013, 2014). Facilitator at New Faculty Workshop (2013-2015) and Future Faculty Workshop (2013-2015)
3. **Advisory:** Member, Sloan MPhD Advisory Committee, Sloan Foundation (2013-2017); Member (2011-2015) and Chair (2016-2017), Cottrell Scholars Advisory Committee, Research Corporation
4. **Promoting Diversity:** Frequent invitations at Colleges, Universities and Public Lectures on the topic of "Advancing Chemistry Through Diversity"
5. **Broad Dissemination:** Blogging on [EveryWhereChemistry.blogspot.com](http://EveryWhereChemistry.blogspot.com) since April 23, 2013, presently with over 60,000 page views.

#### F. Collaborators & Other Affiliations (within the last 5 years)

(i) Collaborators: **OXIDE, Center for Sustainable Nanotechnology, RSA CSC Project, Other Projects:** Dr. Thomas Bartsch (Loughborough U.); Dr. Rosa Benito (U. Politecnica de Madrd); Dr. Karen Bjorkman (U. Toledo); Dr. Karl Booksh (U. Delaware); Dr. Florentino Borondo (U. Autonoma de Madrid); Dr. Iain Boyd (U. Michigan); Dr. Browne Browne (Mount Holyoke); Dr. Gail Burd (U. Arizona); Dr. Erin Carlson (U. Minnesota); Dr. Cristel Chandre (Aix-Marseille U.); Dr. Qian Cui (UW-Madison); Dr. Michael Curry (Tuskegee U.); Dr. Larry Dalton (U. Washington); Dr. Lizanne DeStefano (Georgia Tech); Dr. Frank Dobbin (Harvard U.); Dr. Peter Dorhout (Kansas State U.); Dr. Luis Echegoyen (UTEP); Dr. Charles Eckert (Georgia Tech); Dr. Archie Ervin (Georgia Tech); Dr. Howard Fairborther (Johns Hopkins U.); Dr. Andrew Feig (Wayne State U.); Dr. Vivian Feng (Augsburg College); Dr. Michelle Francl (Bryn Mawr); Dr. Franz Geiger (Northwestern) U.; Dr. Robert Hamers (UW-Madison); Dr. Philip Hammer (American Institute of Physics); Dr. Paula Hammond (MIT); Dr. Ron Hanson (Stanford U.); Dr. Christy Haynes (U. Minnesota); Dr. Malika Jeffries-El (MIT); Dr. Tom Keyes (Boston U); Dr. Rebecca Klaper (UW-Milwaukee); Dr. Charles Liotta (Georgia Tech); Dr. Sara Mason (U. Iowa); Dr. Cathy Murphy (U. Illinois); Dr. Teri Odom (Northwestern U.); Dr. Mary Jo Ondrechen (Northeastern U.); Dr. Galya Orr (PNNL); Dr. Joel Pedersen (UW-Madison); Dr. Eli Pollak (Weizmann Institute); Dr. Stephen Quirk (Kimberly Clark); Dr. Zeev Rosenzweig (UMBC);; Dr. Jennifer Ross (U. Mass. Amherst); Dr. Jennifer Ross (U. Mass. Amherst); Dr. Vincent Rotello (U. Mass. Amherst); Dr. Peter Saalfrank (U.Potsdam); Dr. Gary Schuster (Georgia Tech); Dr. Denise Sekaqueptawa (U. Michigan); Dr. Kyril Solntsev (Georgia Tech); Dr. Marilyn Stains (U. Nebraska Lincoln); Dr. John Stanton (U. Texas Austin); Dr. Jean Stockard (U. Oregon); Dr. Tim Swager (MIT); Dr. Turgay Uzer (Georgia Tech); Dr. Jodi Wesemann (American Chemical Society).

(ii) PI's postdoctoral advisors: Dr. G. A. Voth, U. Utah (1995-96), Dr. E. Pollak, Weizmann Institute (1994).

PI's Ph.D. advisor: Dr. W. H. Miller. U.C., Berkeley (1989-93).