Dr. Robert J. Cave
Curriculum Vitae

Personal

Citizenship: U.S.
Born: June 6, 1957, Brooklyn N.Y.

Professional Background

2016-	Program Director, Chemical Theory, Modeling and Computation, National Science Foundation
2015-16	Associate Dean for Academic Affairs, Harvey Mudd College
2012-13	Visiting Researcher, University of Texas, Austin
2007-12	Vice President for Academic Affairs and Dean of Faculty, Harvey Mudd College
2003-07	Associate Dean for Academic Affairs, Director of Study Abroad, Harvey Mudd College
2001-02	Visiting Professor, Rutgers University
1999-	Professor of Chemistry, Harvey Mudd College
1993-99	Associate Professor of Chemistry, Harvey Mudd College
1994-95	Research Associate, Brookhaven National Laboratory
1993-98	Camille and Henry Dreyfus Teacher-Scholar
1988-92	Assistant Professor of Chemistry, Harvey Mudd College
1985-88	Postdoctoral Fellow, Indiana University; E.R. Davidson, advisor

Education

1986	Ph.D. in Chemistry, California Institute of Technology; R.A. Marcus, W. A. Goddard III, advisors.
1979	B.S. in Chemical Physics, graduated with High Honors, Michigan State University.

Honors and Awards

1993-98	Camille and Henry Dreyfus Teacher-Scholar
1979-82	National Science Foundation Predoctoral Fellow

Professional Affiliations

American Chemical Society

Service to the Professional Community

Editorial Advisory Board Journal of Physical Chemistry 2010-2014

Member of the Executive Committee, Physical Chemistry Division of the ACS term ended 2015.
Co-organizer Gordon Research Conference on Donor-Acceptor Interactions, 2010
Co-organizer of Physical Chemistry Symposia at three ACS National Meetings

Research Interests

Electronic Structure Theory: Development of methods for the theoretical treatment of the electronic coupling element in electron transfer reactions and treatment of electron correlation in atoms and molecules. *Ab initio* studies of electronically excited states of molecules.

Publications

Publications While at Harvey Mudd College (Undergraduate coauthors denoted with a *)

Cave, R.J. "Size-Inconsistency Effects in Molecular Properties for States with Valence-Rydberg Mixing: Low-Lying $\pi \rightarrow \pi^*$ States of Ethylene and Butadiene," *J. Chem. Phys.* **1990**, *92*, 2450.

Anderson; M.A.*; Cave, R.J. "Calculation of Excitation Energies Using Quasidegenerate Variational Perturbation Theory and Multireference-Averaged Coupled-Pair Functional Theory," *Chem. Phys.* **1991**, *154*, 1.

Cave R.J.; Perrott, M.* "Theoretical Investigation of the Ground and Low-Lying Excited States of Butadiene Radical Cation," *J. Chem. Phys.* **1992**, *96*, 3745.

Cave, R.J.; Xantheas, S.; Feller, D. "Exploiting Regularity in Systematic Sequences of Wavefunctions Which Approach the Full CI Limit," *Theor. Chim. Acta.* **1992**, *83*, 31.

Cave, R.J.; Johnson, J.* "A Theoretical Examination of the Rotamers of Hexatriene Radical Cation," *J. Phys. Chem*. **1992**, *96*, 5332.

Dickey, R.P.*; Maurice, D.*; Cave, R.J.; Mawhorter, R. "A Theoretical Investigation of the Geometries, Vibrational Frequencies, and Binding Energies of Several Alkali Halide Dimers," *J. Chem. Phys.* **1993,** *98,* 2182.

Goldstein, E.; Jin, S.; Carrillo, M.R.*; Cave, R.J.; "*Ab Initio* Study of the Ground and Excited States of HCP and its Isomer HPC," *J. Comput. Chem.* **1993,** *14,* 186.

Cave, R.J.; Ono, I.A.* "A Theoretical Investigation of the Geometries, Vibrational Frequencies, and Binding Energies of Several Mixed Alkali Halide Dimers," *J. Chem. Phys.* **1993**, *99*, 9764.

Hong, H.S.* ;Cave, R.J. "A Theoretical Investigation of the Stability of HPC," *J. Phys. Chem.* **1994**, *98*, 10036.

Keszthelyi, T.; Wilbrandt, R.; Cave, R.J.; Johnson, J.L.* "Resonance Raman Investigation of the Radical Cation of 1,3,5-Hexatriene," *J. Phys. Chem.* **1994**, *98*, 5632.

Cave, R.J.; Johnson, J.L.*, Anderson, M.A.* "Calculation of Electric Dipole Transition Moments Using Quasi-Degenerate Variational Perturbation Theory and Averaged Coupled-Pair Functional Theory," *Int. J. Quantum Chem.* **1994**, *50*, 135.

Cave, R.J.; Newton, M.D.; Kumar, K.; Zimmt, M.B. "Theoretical Study of Solvent Effects on the Electronic Coupling Element in Rigidly Linked Donor-Acceptor Systems," *J. Phys. Chem.* **1995,** *99*, 17501.

Cave, R.J.; Newton, M.D. "Generalization of the Mulliken-Hush Treatment for the Calculation of Electron Transfer Matrix Elements," *Chem. Phys. Lett.* **1996**, *249*, 15.

Törring, T.; Biermann, S.; Hoeft, J.; Mawhorter, R.; Cave, R.J.; Szemenyei, C.* "The Structure of Alkali Halide Dimers: A Critical Test of Ionic Models and New *Ab Initio* Results," *J. Chem. Phys.* **1996**, *104*, 8032.

Cave, R.J.; Newton, M.D. "Calculation of Electronic Coupling Matrix Elements for Ground and Excited State Electron Transfer Reactions: Comparison of the Generalized Mulliken-Hush and Block Diagonalization Methods," *J. Chem. Phys.* **1997**, *106*, 9213.

Mawhorter, R.; Cave, R.J.; Pulham, C.; Biermann, S.; Hoeft, J.; Törring, T. "A Harmonic Potential Function for Lithium Sodium DiFlouride," *J. Mol. Struct.* **1997**, *413-414*, 415.

Newton, M.D.; Cave, R.J. "Molecular Control of Electron and Hole Transfer Processes: Theory and Applications," in *Molecular Electronics,* J. Jortner and M. Ratner, eds. (Blackwell, Malden, MA, 1997).

Cave, R.J. "Ab Initio Methods for the Description of Electronically Excited States: Survey of Methods and Select Results," in *Modern Electronic Structure Theory and Applications in Organic Chemistry*, E. R. Davidson, ed. (World, New Jersey, 1997), p. 197.

Henderson, T.M.*; Cave, R.J. "An *Ab Initio* Study of Specific Solvent Effects on the Electronic Coupling Element in Electron Transfer Reactions," *J. Chem. Phys.* **1998**, *109*, 7414.

Hoffman, G.J.; Swafford, L.A.*; Cave, R.J. "An *Ab Initio* Study of the Mono- and

Difluorides of Krypton," *J. Chem. Phys.* **1998**, *109*, 10701.

Miller, N.E.*; Wander, M.C.*; Cave, R.J. "A Theoretical Study of the Electronic Coupling Element for Electron Transfer in Water," *J. Phys. Chem. A*. **1999**, *103*, 1084.

Castner, E.W. Jr.; Kennedy, D.*; Cave, R.J. "Solvent as Electron Donor: Donor/Acceptor Coupling is a Dynamical Variable," *J. Phys. Chem. A* **2000**, *104*, 2869.

Lappe, J.*; Cave, R.J. "On the Vertical and Adiabatic Excitation Energies of the 2^1A(g), State of trans-1,3-butadiene," *J. Phys. Chem. A* **2000**, *104*, 22294.

Cave, R.J; Castner, E. W. Jr. "Time-Dependent Density Functional Theory Investigation of the Ground and Excited States of Coumarins 102, 152, 153, and 343*," J. Phys. Chem. A* **2002**, *106*, 12117.

Cave, R.J.; Burke, K.; Castner, E. W. Jr. "Theoretical Investigation of the Ground and Excited States of Coumarin 151 and Coumarin 120," *J. Phys. Chem. A* **2002**, *106*, 9294.

Cukier, E.*; Daniels, S.*; Vinson, E.*; Cave, R.J. "Are Hydrogen Bonds Unique Among Weak Interactions in Their Ability to Mediate Electronic Coupling?," *J. Phys. Chem. A* **2002**, *106*, 11240.

Rust, M.*; Lappe, J.*; Cave, R. J. "Multistate Effects in Calculations of the Electronic Coupling Element for Electron Transfer using the Generalized Mulliken-Hush Method," *J. Phys. Chem. A* **2002**, *106*, 3930.

Cave, R.J.; Zhang, F.; Maitra, N.T.; Burke, K. "A Dressed TDDFT Treatment of the 2^1Ag states of Butadiene and Hexatriene," *Chem. Phys. Lett.* **2004**, *389*, 39.

Maitra, N.T.; Zhang, F.; Cave, R.J.; Burke, K.; "Double Excitations within Time-Dependent Density Functional Theory Linear Response," *J. Chem. Phys.* **2004**, 120, 5932.

Cukier, E, Cave RJ, "A Comparison of Through-Space and Through-Bond Coupling for Tunneling in Alkane Chains," Cukier, E, Cave RJ, *Chem. Phys. Lett.* **2005,** 402 (1-3): 186.

Lappe, J, Cave, RJ, Newton, MD, Rostov, IV**, "**A Theoretical Investigation of Charge Transfer in Several Substituted Acridinium Ions**,"** *J. Phys. Chem. B.* **2005,** 109 (14): 6610.

Kurlancheek, W.*; Cave, R. J. "Tunneling Through Weak Interactions: "A Comparison of Through-Space-, H-bond-, and Through-Bond-Mediated Tunneling," *J. Phys. Chem A,* **2006**, 110, 14018.

Pheasant, S.*; Kouzelos, J. A.*; Van Ryswyk, H.; Cave, R. J. "Theoretical Investigation of the Electronic Coupling Element in bis-Ruthenium Porphyrin Dimers," *Molec. Simul.* **2006**, 32, 677.

Subotnik, J. E., Yegenah, S., Cave, R. J., Ratner, M. A. "Constructing Diabatic States from Adiabatic States: Extending Generalized Mulliken-Hush to Multiple Charge Centers with Boys Localization," *J. Chem. Phys.* **2008**, 128, 244101.

Cave, R. J. "Inducing Chirality with Circularly Polarized Light," *Science*, **2009**, 323, 1435.

Subotnik, J. E., Cave, R. J., Steele, R. P., Shevni, N. "The Initial and Final States of Electron and Energy Transfer Processes: Diabatization as Motivated by System-Solvent Interactions," *J. Chem. Phys.* **2009**, 130, 234102.

Cave, R. J., Edwards, S. E., Kouzelos, J. A., Newton, M. D. "Reduced Electronic Spaces for Modeling Donor/Acceptor Interactions," *J. Phys. Chem. A,* **2010**, *114*, 14631.

Cave, R.J; Newton, M. D. "Multi-State Treatments of the Electronic Coupling in Donor-Bridge-Acceptor Systems: Insights and Caveats from a Simple Model," *J. Phys. Chem. A,* **2013,** *118,* 7221.

Cave, R. J.; Stanton, J. F.; "Block Diagonalization of the Equation-of-Motion Coupled Cluster Effective Hamiltonian: Treatment of Diabatic Potential Constants and Triple Excitations," *J. Chem. Phys.* **2014,** *140,* 214112.

Hartley, M.K.*; Vine, S.*; Walsh, E.*; Avrantinis, S.*; Daub, G.. W.; Cave, R. J. "Comparison of Relative Activation Energies Obtained by Density Functional Theory and the Random Phase Approximation for Several Claisen Rearrangements," *J. Phys. Chem. B.* **2015**, DOI: 10.1021/acs.jpcb.5b06646.

Cave, R. J.; Stanton, J. F. "A Simple Quasi-diabatization Scheme Suitable for Spectroscopic Problems Based on One-Electron Properties of Interacting States," Cave, R. J.; Stanton, J. F. *J. Chem. Phys.* **2016**. DOI: 10.1063/1.4940426

Postdoctoral Publications

West, P.; Kramer, J.; Baxter, D.V.; Cave, R.J.; Baldeschwieler, J.D. "Chemical Applications of Scanning Tunneling Microscopy," *IBM Journal of Research and Development* **1986**, *30*, 484.

Cave, R.J.; Baxter, D.V.; Goddard, W. A. III; Baldeschwieler J. D. "Theoretical Studies of Electron-Transfer in Metal Dimers," *J. Chem. Phys*. **1987**, *87*, 926.

Cave, R.J.; Davidson, E.R. "A Theoretical Investigation of Some Low-Lying Singlet States of 1,3-Butadiene," *J. Phys. Chem.* **1987**, *91*, 4481.

Cave, R.J.; Davidson, E.R. "A Theoretical Investigation of Several Low-Lying States of *trans, trans* 1,3,5-Hexatriene," *J. Phys. Chem.* **1988**, *92,* 614.

White, J.A.; Cave, R.J.; Davidson, E.R. "An Ab Initio Investigation of the Stabilization of Selected β- and α- substituted Ethyl and Methyl Cations," *J. Am. Chem. Soc.* **1988**, *110*, 6308.

Cave, R.J.; Davidson, E.R. "An Ab Initio Investigation of Several Low-Lying States of all- *trans* Octatetraene," *J. Phys. Chem.* **1988**, *92*, 2173.

Cave, R.J.; Davidson, E.R. "Hylleraas Variational Perturbation Theory: Application to Correlation Problems in Molecular Systems," *J. Chem. Phys*. **1988**, *88*, 5770.

Cave, R.J.; Davidson, E.R. "Ab Initio Estimates of 0-0 Transition Energies in Butadiene and Hexatriene," *Chem. Phys. Lett.*, **1988**, *148*, 190.

Cave, R.J.; Davidson, E.R. "Quasidegenerate Variational Perturbation Theory and the Calculation of First-order Properties from Variational Perturbation Theory Wavefunctions," *J. Chem. Phys.***1988**, *89*, 6798.

Cave, R.J.; Davidson, E.R.; Sautet, P.; Canadell, E.; Eisenstein, E. "A Theoretical Study of Models for X_2Y_2 Zintl Ions," *J. Am. Chem. Soc.* **1989**, *111*, 8105.

Graduate Publications

Allison, J.N.; Cave, R.J.; Goddard, W.A., III "Alkali Oxides. Analysis of Bonding and Explanation of the Reversal of Ordering of the $^2\Sigma$ and $^2\Pi$ States," *J. Phys. Chem*. **1984**, *88*, 1262.

Siders, P.; Cave, R.J.; Marcus, R.A. "A Model for Orientation Effects in Electron-Transfer Reactions," *J. Chem. Phys*. **1984**, *81*, 5613.

Cave, R.J.; Siders, P.; Marcus, R.A. "Mutual Orientation Effects on Electron-Transfer Reactions between Porphyrins," *J. Phys. Chem*., **1986**, *90*, 1436.

Cave, R.J.; Klippenstein, S.J; Marcus, R. A. "A Semiclassical Model for Orientation

Effects in Electron-Transfer Reactions," *J. Chem. Phys*. **1986**, *84*, 3089.

Undergraduate Publications

Guyer, K.L.; Barr, S.W.; Cave, R.J.; Weaver, M.J. `"Electrode Kinetics and Double-Layer Structure at Solid Electrodes," in *Proceedings of the Third Symposium on Electrode Processes, 1979*, eds. S. Bruckenstein *et al.* (The Electrochemical Society, Princeton, N. J. 1980) p. 390.

Yee, E.L.; Cave, R. J.; Guyer, K.L.; Tyma, P.D.; Weaver, M.J. "A Survey of Ligand Effects Upon the Reaction Entropies of Some Transition Metal Redox Couples," *J. Am. Chem. Soc.*, **1979**, *101,* 1131.

Research Presentations (while at Harvey Mudd College, not including student presentations)

"Ab Initio Studies of Polyene Electronic Spectra," University of California Riverside, February, 1990; talk.

"Application of QuasidegenerateVariational Perturbation Theory to the Calculation of Electronic Excitation Energies," Twelfth Annual West Coast Theoretical Chemistry Conference, 1990; poster.

"A Theoretical Investigation of the Low-Lying States of Butadiene Radical Cation," American Conference on Theoretical Chemistry, 1990; talk.

"Ab Initio Studies of the Ground and Excited States of Molecules," California Polytechnic University at Pomona, May 1991; talk.

"A Theoretical Investigation of the Low-Lying States of Butadiene Radical Cation," VIIth International Conference on Quantum Chemistry," Menton, France, July 1991, poster.

"A Theoretical Investigation of the Low-Lying States of Butadiene Radical Cation," National ACS Meeting, New York, August 1991, poster.

"Application of Approximately Size-Consistent Methods to the Study of Molecular Excited States," National ACS Meeting, San Francisco, April 1992, invited talk.

"A Theoretical Investigation of Several Low-Lying States of CH_2NH and CH_2NH^+," West Coast Conference on Theoretical Chemistry, June, 1993; poster.

"A Theoretical Investigation of Several Low-Lying States of CH_2NH and CH_2NH^+," American Conference on Theoretical Chemistry, June, 1993; poster.

"Methods for the Calculation of the Electronic Coupling Element in Electron Transfer Reactions," Dept. Of Chemistry, Brookhaven National Laboratory, February 1995; talk.

"Methods for the Calculation of the Electronic Coupling Element in Electron Transfer Reactions," Dept. Of Chemistry, Columbia University, April 1995; talk.

"Methods for the Calculation of the Electronic Coupling Element in Electron Transfer Reactions," Dept. Of Energy Solar Photochemistry Conference, June 1995; poster.

"Theoretical Studies of Electron Transfer Processes: Ab Initio Studies of Solvent Effects on the Electronic Coupling Element," American Conference on Theoretical Chemistry, June, 1996; poster.

"Theoretical Studies of Electron Transfer Processes: Ab Initio Studies of Solvent Effects on the Electronic Coupling Element," Electron Donor-Acceptor Interactions Gordon Conference, August, 1996; invited talk.

"Theoretical Studies of Electron Transfer Processes: Ab Initio Studies of Solvent Effects on the Electronic Coupling Element," National ACS Meeting, San Francisco, April 1997; talk.

"Solvent Effects on the Electronic Coupling Element in Electron transfer Reactions," *Oesper Symposium*, University of Cincinnati, October 1997; talk.

Theoretical Studies of Solvent Effects on Electron Transfer Reactions, Colorado State University, March 1998; talk.

Theoretical Studies of Solvent Effects on Electron Transfer Reactions, ACS Spring Meeting, Dallas, 1998; poster.

"Ultrafast Photo-Induced Electron Transfer from Solvent: Inertial Solvent Dynamics and Electronic Coupling," ACS Spring Meeting, Dallas, 1998; talk (with E. Castner).

"What is β in Water?" Electron Donor-Acceptor Interactions Gordon Conference, Newport Rhode Island, August, 1998; poster.

"Solvent Effects on Electron Transfer Reaction," University of Florida, Gainseville, November 1998; talk.

"Solvent Effects on Electron Transfer Reaction," California State University, Long Beach, October 1999; talk

"Methods for Calculating the Electronic Coupling Element for Electron Transfer Reactions," Nonadiabatic Dynamics Workshop, Telluride, CO, July 30-August 5, 2000; talk.

"Correlation and Multi-State Effects on the Electronic Coupling Element for Electron Transfer Reactions," Spring ACS Meeting, 2001; poster.

"Solvent Effects on the Electronic Coupling Element for Electron Transfer Reactions," Rutgers University, Fall, 2001, talk.

Poster on Solvent Effects on Electronic Coupling, Electron Donor-Acceptor Interactions Gordon Conference, Newport Rhode Island, August, 2002.

"TDDFT study of the Low-Lying Excited States of Coumarins 102, 152, 153, and 343" (E. W. Castner co-author), ACS Spring Meeting, New Orleans, LA, Spring 2003.

"A Comparison of Through-Space and Through-Bond Coupling for Tunneling in Alkane Chains," Electron Donor-Acceptor Interactions Gordon Conference, Newport Rhode Island, August, 2004; poster.

"Theoretical Studies of the Electronic Coupling Element for Electron Transfer Reactions." American Conference on Theoretical Chemistry, (July 2005), Talk.

"Ab Initio Calculation of Local Electronic Coupling Elements – Some Bad News," ACS Physical Chemistry Symposium, "20 Years of Pathways, ACS Spring Meeting, Anaheim, CA, March 2011.

"The Electronic Coupling Element in Electron Transfer Reactions: A Sensitive Probe of Bonding and Dynamics." Sanibel Meeting, (February 2012), Talk.

"What Makes For Fast Electron Transfer In Biology, And Why Should You Care? One Theorist's Point Of View." Elisheva Goldstein Memorial Lecture, Cal Poly Pomona, (May 2013), Talk.

"Block Diagonalization Approach to Diabatic EOM-CC States." ACS Meeting, Dallas (March 2014), Talk.

"Diabatic States for Spectroscopy and Electron Transfer Processes." University of California, Irvine, (April 2014), Talk.

"Quasidiabatization Methods for Spectroscopy and Charge Transfer." "The Batsheva de Rothschild Seminar on Molecular Electronics 2015: 40 years later." Poster.

"Butadiene – the simplest of polyenes? Not by a long shot." Pacifichem, December 2015, Invited Talk.

"Quantum Chemical Alchemy: Dynamical Gold from Born-Oppenheimer Lead." University of California, Davis (April 2016), Talk.

Sources of External Funding

Petroleum Research Fund: Two year, type G starter grant for $18,000. "Theoretical Studies of Gas-Phase Energy Transfer." 1989-1992.

National Science Foundation Instrumentation and Laboratory Improvement Grant: Two year grant for $53,500. "A Center for Computational Chemistry." Co-PI, 1989-1992.

National Science Foundation Research in Undergraduate Institutions Grant: Two year grant for $50,000. "A Theoretical Investigation of Molecular Excited States." 1990-1992.

Western Cluster Pew Science Program Collaborative Research Grant (with Richard J. Mawhorter, Pomona College): One year grant for $10,000. "The Problem of the Alkali Halide Dimer Structures: An Integrated Multidisciplinary Approach." 1990-1991.

National Science Foundation Research in Undergraduate Institutions Grant: Three year grant for $129,000. "A Theoretical Investigation of Molecular Ground and Excited States." 1993-1997.

Camille and Henry Dreyfus Teacher-Scholar Award, $60,000. 1993-1998.

National Science Foundation Academic Research Infrastructure Grant: One year grant for $105,000. "Acquisition of a Multi-Purpose Facility for Computational Chemistry." 1995-97.

Petroleum Research Fund Type B Grant: Two year grant for $25,000. "Theoretical Investigations of Electronic Coupling Elements in Electron Transfer Reactions." 1997-99.

National Science Foundation Research in Undergraduate Institutions Grant: Three year grant for $142,700. "Theoretical Investigation of Electronic Coupling Elements in Electron Transfer Reactions." 1998-2001.

National Science Foundation Research Experiences for Undergraduates Grant: Three year grant for $123,000, "National Science Foundation Research Experiences for Undergraduates at Harvey Mudd College." 1998-2000.

Petroleum Research Fund Type B Grant: Two year grant for $30,000. "Electron Correlation Effects on the Electronic Coupling Element for Electron Transfer Reactions." 2000-02.

Petroleum Research Fund Type B Grant: Three year grant for $50,000. "Theoretical Studies of

the Electronic Coupling Element in Electron Transfer Reactions." 2002-05.

National Science Foundation Research in Undergraduate Institutions Grant: Three year grant for $255,000. "Experimental and Theoretical Investigations of Electronic Coupling in Metalloporphyrin Dimers and Trimers," (H. Van Ryswyk and R. J. Cave co-PIs). 2004-2007.

National Science Foundation Research in Undergraduate Institutions Grant: Three year grant for $ 261,078. "Correlated Methods for Calculation of the Electronic Coupling Element," 2016-2019.