Anthony D. Dutoi

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Professional Experience

University of the Pacific, Stockton, California — Aug. 2012 – present

- Assistant Professor

Ruprecht-Karls-Universität Heidelberg, Germany — Apr. 2008 – Jul. 2012

- Postdoctoral research with Lorenz S. Cederbaum
- Tracing of electronic excitation dynamics in real time and space using propagator methods

Northwestern University, Evanston, Illinois — Aug. 2006 – Mar. 2008

- Postdoctoral research with Tamar Seideman
- Development of flexible grid-based wavefunction propagations for bound–unbound transitions

Education

Ph.D. in Chemistry – University of California, Berkeley — May 2006

- Thesis Title: *Novel Approaches to Solving the Electronic Schrödinger Equation for Molecules*
- Advisor: Martin Head-Gordon

B.S. in Chemistry – Saint Louis University, St. Louis, Missouri — May 1999

- Thesis Title: *A Molecular Orbital Analysis of the Geometry of Amines and Phosphines*
- Advisor: Ronald F. See

Courses Taught

Quantum Mechanics (undergraduate)	Pacific (Spring 2015)
Molecular Spectroscopy (graduate)	Pacific (Fall 2014)
General Chemistry I	Pacific (6 semesters, 2012 – present)
General Chemistry II	Pacific (2 semesters, 2014 – present)
Teaching and Learning Chemistry (for Workshop leaders)	Pacific (2 semesters, 2015 – present)
Overview of Electronic Structure Methods (unofficial)	Northwestern (2007), Heidelberg (2009)
Discussion instructor: Quantum Mechanics, Biophysical Chemistry	Berkeley (1 semester each)
Laboratory instructor: General Chemistry	Saint Louis (6 semesters), Berkeley (1 semester)

Funding and Honors

Visiting Faculty Program at Berkeley National Laboratory (summer salary, 2014, 2015)

Pacific Fund Grants (internal competition):
$2000 for storage server, Undergrad summer support (1), Graduate conference attendance (1)

University of the Pacific Hornage Fund ($45,000 start-up)

German Science Foundation (DFG) project funding
(2011–2012, postdoc salary for 2 years, graduate student for 3 years, plus travel)

Humboldt Fellowship for research at the Universität Heidelberg (2008 – 2010)

Fulbright Grant for study at the Universität Göttingen (1999 – 2000)

University Scholarship at Saint Louis University (1995 – 1999, $5500 each year)

Outstanding Senior (1999) and Junior (1998) in Chemistry at Saint Louis University

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Languages

English: Mother tongue

German: Professional working proficiency (approximately S-3 level)

Professional Societies

American Chemical Society member (since 2007)

American Physical Society member (since 2007)

Professional Service

Editorial Board Member for *Scientific Reports*, 2014–2016 (open access, Nature Publishing Group)

Peer reviewer for: *Journal of Physical Chemistry*, *Journal of Physical Chemistry Letters*, *Journal of Chemical Physics* (also *Communications*), *Chemical Physics*, *Chemical Physics Letters*, *Molecular Physics*, *Journal of Chemical Theory and Computation*, *Journal of Computational Chemistry*, *Journal of Physics B (Atomic, Molecular and Optical Physics)*, *Frontiers in Theoretical and Computational Chemistry*

Chair of the session "Electron Correlation Theory/Linear Scaling" at the 2011 Congress of the World Association of Theoretical and Computational Chemists

Organizer of University of the Pacific Chemistry Department Seminars, 2014–2015

Faculty scientific advisor for UOP's all-female High-performance Computing Challenge Team, 2013 (second place in competition for the application category for which I was advising)

Coordinated purchase of new Chemistry Department computational cluster, 2015

Met with developers of `www.gradescope.com` (grading software, free use) to give feedback and contribute sample code, 2015

Participant in the Director's Review of Lawrence Berkeley National Laboratory (2006, in lieu of Martin Head-Gordon)

University Committees and Task Forces:

- "Pacific Seminar I" Planning Committee (Spring 2013)
- Technology in Education Committee (Spring 2014 – Spring 2015)
- *Ad Hoc* Learning Management System Review Task Force (Spring 2015)
- Academic Affairs Committee (Fall 2015)
- *Ad Hoc* Faculty Compensation Task Force (Spring 2016 – Spring 2017)

Dissertation Committees:

- Sampada Borkar, (Ph.D., 2012, University of the Pacific, B. Sztaray)
- Chrissa Mozaffari, (Ph.D., *pending*, University of the Pacific, B. Sztaray)
- Kyle Covert, (Ph.D., *pending*, University of the Pacific, B. Sztaray)
- Zufan Wu, (Ph.D., *pending*, University of the Pacific, J. Ren)
- Michael Pastor, (Ph.D., *pending*, University of the Pacific, Q. Zhao)

Academic Outreach

Observer (2015) and future presenter (2016) in MASTER project of the Lincoln Unified School District (K-8th grade), funded by the California Mathematics and Science Partnership

Facilitated participation of UOP student groups in Science Night of a local elementary school.

Current Research Group

Yuhong Liu (Ph.D. Chemistry)

Boris Daniel Gutiérrez Cortés (Ph.D. Chemistry)

Johnson Liu (B.S. Chem., mentored application for Goldwater Scholarship and REU programs)

Josiah Yoshimura (B.S. Comp. Sci., mentored application to REU programs)

Past Group Members

Zubair Amin (undergraduate)

Kyu-Ri Li (undergraduate)

PEER-REVIEWED PUBLICATIONS

23) Y. Shao, Z. Gan, E. Epifanovsky, A. T. B. Gilbert, M. Wormit, J. Kussmann, A. W. Lange, A. Behn, J. Deng, X. Feng, D. Ghosh, M. Goldey, P. R. Horn, L. D. Jacobson, I. Kaliman, R. Z. Khaliullin, T. Kuś, A. Landau, J. Liu, E. I. Proynov, Y. M. Rhee, R. M. Richard,M. A. Rohrdanz, R. P. Steele, E. J. Sundstrom, H. L. Woodcock III, P. M. Zimmerman, D. Zuev, B. Albrecht, E. Alguire, B. Austin, G. J. O. Beran, Y. A. Bernard, E. Berquist, K. Brandhorst, K. B. Bravaya, S. T. Brown, D. Casanova, C.-M. Chang, Y. Chen, S. H. Chien, K. D. Closser, D. L. Crittenden, M. Diedenhofen, R. A. DiStasio Jr., H. Do, **A. D. Dutoi**, R. G. Edgar, S. Fatehi, L. Fusti-Molnar, A. Ghysels, A. Golubeva-Zadorozhnaya, J. Gomes, M. W. D. Hanson-Heine, P. H. P. Harbach, A. W. Hauser, E. G. Hohenstein, Z. C. Holden, T.-C. Jagau, H. Ji, B. Kaduk, K. Khistyaev, J. Kim, J. Kim, R. A. King, P. Klunzinger, D. Kosenkov, T. Kowalczyk, C. M. Krauter, K. U. Lao, A. Laurent, K. V. Lawler, S. V. Levchenko, C. Y. Lin, F. Liu, E. Livshits, R. C. Lochan, A. Luenser, P. Manohar, S. F. Manzer, S.-P. Mao, N. Mardirossian, A. V. Marenich, S. A. Maurer, N. J. Mayhall, E. Neuscamman, C. M. Oana, R. Olivares-Amaya, D. P. O'Neill, J. A. Parkhill, T. M. Perrine, R. Peverati, A. Prociuk, D. R. Rehn, E. Rosta, N. J. Russ, S. M. Sharada, S. Sharma, D. W. Small, A. Sodt, T. Stein, D. Stück, Y.-C. Su, A. J. W. Thom, T. Tsuchimochi, V. Vanovschi, L. Vogt, O. Vydrov, T. Wang, M. A. Watson, J. Wenzel, A. White, C. F. Williams, J. Yang, S. Yeganeh, S. R. Yost, Z.-Q. You, I. Y. Zhang, X. Zhang, Y. Zhao, B. R. Brooks, G. K. L. Chan, D. M. Chipman, C. J. Cramer, W. A. Goddard III, M. S. Gordon, W. J. Hehre, A. Klamt, H. F. Schaefer III, M. W. Schmidt, C. D. Sherrill, D. G. Truhlar, A. Warshel, X. Xu, A. Aspuru-Guzik, R. Baer, A. T. Bell, N. A. Besley, J.-D. Chai, A. Dreuw, B. D. Dunietz, T. R. Furlani, S. R. Gwaltney, C.-P. Hsu, Y. Jung, J. Kong, D. S. Lambrecht, W. Liang, C. Ochsenfeld, V. A. Rassolov, L. V. Slipchenko, J. E. Subotnik, T. Van Voorhis, J. M. Herbert, A. I. Krylov, P. M. W. Gill, M. Head-Gordon, "Advances in Molecular Quantum Chemistry contained in the Q-Chem 4 Program Package" *Mol. Phys.* v. 113, p. 184–215 (2015)

22) **A. D. Dutoi** and L. S. Cederbaum, "Time-resolved Pump-Probe Spectroscopy to Follow Valence Electronic Motion in Molecules: Application," *Phys. Rev. A* v. 90, p. 023414-1–023414-21 (2014)

21) **A. D. Dutoi** "Visualising Many-body Electron Dynamics using One-body Densities and Orbitals," *Mol. Phys.* v. 112, p. 1–11 (2014)
Invited article, Author profile: p. 12–13; Also the cover article.
An image from this article was featured as the "back scatter" in Physics Today ***67****-6 68 (2014).*

20) **A. D. Dutoi**, K. Gokhberg and L. S. Cederbaum, "Time-resolved Pump-Probe Spectroscopy to Follow Valence Electronic Motion in Molecules: Theory," *Phys. Rev. A* v. 88, p. 013419-1–013419-17 (2013)

19) M. Goldey, **A. Dutoi** and M. Head-Gordon, "Attenuated Second-order Møller-Plesset Perturbation Theory: Performance within the aug-cc-pVTZ Basis," *Phys. Chem. Chem. Phys.* v. 15, p. 15869–15875 (2013)

18) **A. D. Dutoi** and L. S. Cederbaum, "An Excited Electron Avoiding a Positive Charge," *J. Phys. Chem. Lett.* v. 2, p. 2300–2303 (2011)
Featured in News & Views, Nat. Chem. *v. 4, p. 8 (2012)*

17) **A. D. Dutoi**, M. Wormit and L. S. Cederbaum, "Ultrafast Charge Separation Driven by Differential Particle and Hole Mobilities," *J. Chem. Phys.* v. 134, p. 024303-1–024303-9 (2011)

16) **A. D. Dutoi**, L. S. Cederbaum, M. Wormit, J. H. Starcke and A. Dreuw, "Tracing Molecular Electronic Excitation Dynamics in Real Time and Space," *J. Chem. Phys.* v. 132, p. 144302-1–144302-18 (2010)

PEER-REVIEWED PUBLICATIONS (CONTINUED)

15) A. Dreuw, J. Plötner, M. Wormit, M. Head-Gordon and **A. D. Dutoi**, "An Additive Long-range Potential to Correct for the Charge-transfer Failure of Time-dependent Density Functional Theory," in *Progress in Physical Chemistry* ed. F. M. Dolg, v. 3, p. 21 (Oldenbourg, Munich, 2010)

14) A. Dreuw, J. Plötner, M. Wormit, M. Head-Gordon and **A. D. Dutoi**, "An Additive Long-range Potential to Correct for the Charge-transfer Failure of Time-dependent Density Functional Theory," *Z. Phys. Chem.* v. 224, p. 311–324 (2010)

13) S. Ramakrishna, P. A. J. Sherrat, **A. D. Dutoi** and T. Seideman, "Origin and Implication of Ellipticity in High-order Harmonic Generation from Aligned Molecules," *Phys. Rev. A* v. 81, p. 021802-1–021802-4 (2010)

12) J. A. Parkhill, J.-D. Chai, **A. D. Dutoi**, and M. Head-Gordon, "The Exchange Energy of a Uniform Electron Gas Experiencing a New, Flexible Range Separation," *Chem. Phys. Lett.* v. 478, p. 283–286 (2009)

11) **A. D. Dutoi** and M. Head-Gordon, "A Study of the Effect of Attenuation Curvature on Molecular Correlation Energies by Introducing an Explicit Cutoff Radius into Two-electron Integrals," *J. Phys. Chem. A* v. 112, p. 2110–2119 (2008, William A. Lester Festschrift)

10) Y. Shao, L. F. Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S. T. Brown, A. T. B. Gilbert, L. V. Slipchenko, S. V. Levchenko, D. P. O'Neill, R. A. DiStasio Jr., R. C. Lochan, T. Wang, G. J. O. Beran, N. A. Besley, J. M. Herbert, C. Y. Lin, T. Van Voorhis, S. H. Chien, A. Sodt, R. P. Steele, V. A. Rassolov, P. E. Maslen, P. P. Korambath, R. D. Adamson, B. Austin, J. Baker, E. F. C. Byrd, H. Dachsel, R. J. Doerksen, A. Dreuw, B. D. Dunietz, **A. D. Dutoi**, T. R. Furlani, S. R. Gwaltney, A. Heyden, S. Hirata, C.-P. Hsu, G. Kedziora, R. Z. Khalliulin, P. Klunzinger, A. M. Lee, M. S. Lee, W. Liang, I. Lotan, N. Nair, B. Peters, E. I. Proynov, P. A. Pieniazek, Y. M. Rhee, J. Ritchie, E. Rosta, C. D. Sherrill, A. C. Simmonett, J. E. Subotnik, H. L. Woodcock III, W. Zhang, A. T. Bell, A. K. Chakraborty, D. M. Chipman, F. J. Keil, A. Warshel, W. J. Hehre, H. F. Schaefer III, J. Kong, A. I. Krylov, P. M. W. Gill and M. Head-Gordon, "Advances in Methods and Algorithms in a Modern Quantum Chemistry Program Package," *Phys. Chem. Chem. Phys.* v. 8, p. 3172–3191 (2006)

9) **A. D. Dutoi** and M. Head-Gordon, "Self-interaction Error of Local Density Functionals for Alkali-halide Dissociation," *Chem. Phys. Lett.* v. 422, p. 230–233 (2006)

8) J. E. Subotnik, **A. D. Dutoi** and M. Head-Gordon, "Fast, Localized, Orthonormal Virtual Orbitals which Depend Smoothly on Nuclear Coordinates," *J. Chem. Phys.* v. 123, p. 114108-1–114108-9 (2005)

7) A. Aspuru-Guzik,* **A. D. Dutoi**,* P. J. Love and M. Head-Gordon, "Simulated Quantum Computation of Molecular Energies," *Science* v. 309, p. 1704–1707 (2005)
* *Equal authorship*

6) P. E. Maslen, **A. D. Dutoi**, M. S. Lee, Y. Shao and M. Head-Gordon, "Accurate Local Approximations to the Triples Correlation Energy: Formulation, Implementation and Tests of 5th-order Scaling Models," *Mol. Phys.* v. 103, p. 425–437 (2005)

5) **A. D. Dutoi**, Y. Jung and M. Head-Gordon, "An Orbital-based Definition of Radical and Multiradical Character," *J. Phys. Chem. A* v. 108, p. 10270–10279 (2004)

4) Y. Jung, R. C. Lochan, **A. D. Dutoi** and M. Head-Gordon, "Scaled Opposite-spin Second-order Møller-Plesset Correlation Energy: An Economical Electronic Structure Method," *J. Chem. Phys.* v. 121, p. 9793–9802 (2004)

PEER-REVIEWED PUBLICATIONS (CONTINUED)

3) P. Botschwina, **T. Dutoi**, M. Mladenovic, R. Oswald, S. Schmatz and H. Stoll, "Theoretical Investigations of Proton-bound Cluster Ions," *Faraday Discuss.* v. 118, p. 433–453 (2001)

2) R. F. See, **A. D. Dutoi**, K. W. McConnell and R. M. Naylor, "Geometry of Simple Molecules: Nonbonded Interactions and Not-bonding Orbitals Primarily Determine Observed Geometries," *J. Am. Chem. Soc.* v. 123, p. 2839–2848 (2001)

1) R. F. See, **A. D. Dutoi**, J. C. Fettinger, P. J. Nicastro and J. W. Ziller, "The Crystal Structures of (p-ClPh)$_3$PO and (p-OMePh)$_3$PO, Including an Analysis of the P-O Bond in Triarylphosphine Oxides," *J. Chem. Crystallogr.* v. 28, p. 893–898 (1998)

INVITED TALKS

Oct. 2015, Linac Coherent Light Source Users' Meeting, SLAC, Stanford, California: "Time-resolved Pump–Probe Spectroscopy to Follow Valence Electronic Motion in Molecules: Theory and Simulation"

May. 2014, Facultad de Química, Universidad Nacional Autónoma de México: "Time-resolved Pump–Probe Spectroscopy to Follow Valence Electron Motion"

Jul. 2012, Buchleitner research group meeting, Universität Freiburg, Germany: "Time-resolved Pump–Probe Spectroscopy to Follow Valence Electron Motion"

Aug. 2011, Physical Chemistry Seminar, University of Pennsylvania, Philadelphia: "Time-resolved Pump–Probe Spectroscopy to Follow Valence Electron Motion"

Aug. 2011, Aspuru-Guzik research group meeting, Harvard, Cambridge, Massachusetts: "Time-resolved Pump–Probe Spectroscopy to Follow Valence Electron Motion"

Sep. 2010, Workshop on Self-consistent Green's Function Methods, Commissariat à l'Énergie Atomique, Saclay, France: "Electronic Excitations in Real Time and Space using the Polarization Propagator"
In lieu of Prof. Em. Jochen Schirmer

Jul. 2008, German Science Foundation Graduate School Seminar, Universität Göttingen, Germany: "Practical Limitations of Modern Density-functional Models, Especially Regarding Self-interaction Error"

May 2008, Theory groups' meeting, Università degli Studi, Milan, Italy: "The Electron Dynamics behind High-harmonic Generation: Effective Potentials and Multi-center Interference"

Feb. 2008, Theory groups' meeting, University of Michigan, Ann Arbor: "The Electron Dynamics behind High-harmonic Generation: Focus on Multi-center Interference"

Oct. 2007, Physical Chemistry Seminar, Universität Frankfurt, Germany: "The Electron Dynamics behind High-harmonic Generation: Focus on Multi-center Interference"

Apr. 2007, Aspuru-Guzik research group meeting, Harvard, Cambridge, Massachusetts: "Computational Study of Orientation-dependent Molecular High-harmonic Spectra"

Jul. 2004, Theory groups' meeting, Universität Frankfurt, Germany: "Preventing Electrons from Repelling Themselves in TD-DFT: One Application of a New Integral"

Mar. 1999, St. Louis Rubber Group Meeting (scholarship award), St. Louis, Missouri: "A Molecular Orbital Analysis of the Geometry of Amines and Phosphines"

CONTRIBUTED TALKS

Aug. 2014, Q-Chem Developer Workshop, Berkeley, California: "Q-Chem: The Electronic Structure Theorists' Electronic Structure Code (without ditching present market share)"

Sep. 2013, American Chemical Society Meeting, Indianapolis, Indiana: "Time-resolved Pump-Probe Spectroscopy to Follow Valence Electronic Motion"

Aug. 2011, American Chemical Society Meeting, Denver, Colorado: "Coherence of Particles and Holes in Excitation Migration: A Density-matrix Analysis"
Personally invited by organizers to contribute

CONTRIBUTED TALKS (CONTINUED)

Jul. 2011, 9th Congress of the World Association of Theoretical and Computational Chemists, Santiago de Compostela, Spain: "Time-resolved Pump–Probe Spectroscopy to Follow Valence Electron Motion"

Sep. 2010, Ψ_k Conference, Berlin, Germany: "Tracing Electronic Dynamics of Molecules in Real Time and Space: A Study of Excitation Transfer and Charge Separation"

Jul. 2010, 37th International Conference on Vacuum Ultraviolet and X-ray Physics, Vancouver, Canada: "Tracing Molecular Excitation Dynamics in Real Time and Space"

Sep. 2009, 45th Symposium on Theoretical Chemistry: Excited States, from Photophysics to Photobiology, Neuss, Germany: "Tracing Molecular Excitation Dynamics in Real Time and Space"

Mar. 2009, Deutsche Forschungsgemeinschaft Priority Program Workshop: Recent Advances in Efficient Electron Correlation Methods, Bensberg, Germany: "A Study of the Effect of Attenuation Curvature on Molecular Correlation Energies by Introducing an Explicit Cutoff Radius into Two-electron Integrals"

Mar. 2007, Symposium in Honor of Bill Lester's 70th Birthday, Berkeley, California: "Computational Study of Orientation-dependent Molecular High-harmonic Spectra"

Mar. 2007, American Physical Society Meeting, Denver, Colorado: "Computational Study of Orientation-dependent Molecular High-harmonic Spectra"

Sep. 2006, American Chemical Society Meeting, San Francisco, California: "Inclusion of Long-range Exchange in TD-DFT: Towards a Quantitative Charge-transfer Model"

Feb. 2006, Southwest Quantum Information and Technology meeting, Albuquerque, New Mexico: "Quantum Computation for Quantum Chemistry: Electronic Structure Calculations using Quantum Algorithms"

POSTER PRESENTATIONS

Aug. 2015, American Chemical Society Meeting, Boston, Massachusetts: "Systematically Improvable Exciton Hamiltonians in Large-scale Electronic Structure Calculations" (poster of graduate student Yuhong Liu)

Aug. 2014, American Chemical Society Meeting, San Francisco, California: "Separating Electron Correlations by Energy Scale: A Systematically Improvable Fragment-based Approach" (poster of graduate student Yuhong Liu)

Aug. 2014, American Chemical Society Meeting, San Francisco, California: "Simulating Transient Absorption Spectra using Extremely Broad X-ray Pulses"

Jul. 2014, American Conference on Theoretical Chemistry, Telluride, Colorado: "Time-resolved Spectroscopy to Follow Electronic Motion in Molecules: A Study of Molecular Alignment"

Aug. 2011, American Chemical Society Meeting, Denver, Colorado: "Time-resolved Pump–Probe Spectroscopy to Follow Valence Electron Motion"

Jul. 2011, 27th International Conference on Photonic, Electronic and Atomic Collisions, Belfast, Northern Ireland: "Time-resolved Pump–Probe Spectroscopy to Follow Valence Electron Motion"
Presented by co-author Kirill Gokhberg in my absence

POSTER PRESENTATIONS (CONTINUED)

Jul. 2011, Femto 10, Madrid, Spain: "Time-resolved Pump–Probe Spectroscopy to Follow Valence Electron Motion"

Sep. 2010, 46$^{\text{th}}$ Symposium on Theoretical Chemistry: Quantum Chemistry for Large and Complex Systems, From Theory to Algorithms and Applications, Münster, Germany: "Tracing Molecular Electronic Excitations in Real Time and Space"

Jul. 2010, Ultrafast Spectroscopy Satellite Meeting of the 37$^{\text{th}}$ International Conference on Vacuum Ultraviolet and X-ray Physics, Palo Alto, California: "Tracing Molecular Excitation Dynamics in Real Time and Space"

May 2010, Molecular Quantum Mechanics: An International Conference in Honor of Henry F. Schaefer III, Berkeley, California: "Tracing Electronic Dynamics of Molecules in Real Time and Space: A Study of Excitation Transfer and Charge Separation"

Apr. 2010, First Principles Quantum Chemistry, from Elementary Reactions to Enzymes: An International Conference in Honour of Hans-Joachim Werner's 60th Birthday, Bad Herrenalb, Germany: "Tracing Molecular Electronic Excitation Dynamics in Real Time and Space"

Jul. 2009, 13$^{\text{th}}$ International Conference on Quantum Chemistry, Helsinki, Finland: "Tracing Ultrafast Molecular Electronic Energy Transfer in Real Time and Space"
Poster prize winner (one of three prizes for ca. 300 posters)

Oct. 2008, Humboldt Netzwerk Meeting, Darmstadt, Germany: "Tracing Ultrafast Molecular Electronic Energy Transfer in Real Time and Space"

Aug. 2007, Gordon Research Conference on Quantum Control of Light and Matter, Newport, Rhode Island: "The Electron Dynamics behind Molecular High-harmonic Generation"

Aug. 2007, 13$^{\text{th}}$ International Conference on Unconventional Photoactive Systems, Evanston, Illinois: "The Electron Dynamics behind Molecular High-harmonic Generation"

Jul. 2005, American Conference on Theoretical Chemistry, Los Angeles, California: "An Improved Hybrid Exchange Kernel for Charge-Transfer States in TD-DFT"

Jul. 2004, Molecular Quantum Mechanics: An International Conference in Honor of Nicholas C. Handy, Cambridge, England: "An Orbital-based Definition of Radical and Multiradical Character"

Jul. 2003, XI$^{\text{th}}$ International Conference on Quantum Chemistry, Bonn, Germany: "Structure and Analysis of Wavefunctions"

Jul. 2001, Molecular Quantum Mechanics: An International Conference in Honor of Ernest R. Davidson, Seattle, Washington: "An Accurate Local Model for Triple Substitutions"

Jul. 1997, Annual Meeting of the American Crystallographic Association, St. Louis, Missouri: "A Molecular Orbital Analysis of the Geometry of Amines and Phosphines"