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CURRICULUM VITAE

RODNEY J. BARTLETT

GRADUATE RESEARCH PROFESSOR OF CHEMISTRY AND PHYSICS
QUANTUM THEORY PROJECT
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BIRTH DATE: March 31, 1944

CV INDEX

AREA OF SPECIALIZATION

Quantum chemistry, molecular electronic structure and spectra, *ab initio* many-electron methods

Following the initial formulation of Jiri Cizek of coupled-cluster theory with double excitations, CCD, Rod Bartlett pioneered the development of coupled-cluster (CC) theory in quantum chemistry to offer highly accurate solutions of the Schroedinger equation for molecular structure and spectra. He introduced the term 'size-extensivity' for many-body methods like CC that scale properly with the number of electrons; now viewed as an essential element in quantum chemistry approximations. He and his co-workers were the first to formulate and implement CC theory with all single and double excitations (CCSD), to add triples non-iteratively (CCSD[T]), iteratively, CCSDT-1, and fully, CCSDT; followed by quadruple (CCSDTQ) and pentuple excitations (CCSDTQP). He also presented a density matrix formulation for the analytical gradients (forces) for the non-variational CC method, a necessity for any widely used method in quantum chemistry. This led to the CC functional, $E=\langle 0|(1+X)\exp(-T)H\exp(T)|0\rangle$ where the forces on an atom, α, become $\partial E/X_\alpha=\langle 0|(1+X)\exp(-T)(\partial H/\partial X_\alpha)\exp(T)|0\rangle$. This functional also defines the CC response and relaxed density matrices for all properties, a non-Hermitian generalization of the conventional density matrices. With energies, analytical forces, excited states, density matrices, and other properties, CC theory has now been documented to offer the most predictive, widely applicable, results in the field. Hence, Bartlett has been instrumental in establishing the now well-accepted paradigm MP2<CCD<CCSD<CCSD(T)<CCSDT<CCSDT(Q_f)<CCSDTQ<Full CI, for

converging, many-body, quantum chemical methods. The history is summarized in the article, ""How and Why Coupled-cluster Theory Become the Pre-eminent *Ab Initio* Method in Quantum Chemistry?" in *Theory and Applications of Computational Chemistry: The First Forty Years,* (C. Dykstra, G. Frenking, K. Kim and G. Scuseria, editors) Elsevier, 1191-1221 (2005).

His group is also responsible for the widely used ACES II program system. He is the author of 39 book chapters and 527 journal articles.

Other research topics include:

- The search for metastable, high-energy density molecules (HEDM) like N_4 N_8, and N_5^-, which he has long predicted to exist (The pentazole anion, an aromatic five-membered ring, was recently observed for the first time in negative ion mass spectra and in solution by NMR, verifying his prediction).
- Non-linear optical properties of molecules, where his work resolved long-standing discrepancies between theory and electric-field induced second and third harmonic generation experiments. The new theory produced in this work introduced any-order time-dependent Hartree-Fock theory for frequency dependent properties and that for the initial time-dependent CC results.
- Carbon clusters, where his work on the rhombic form of C_4, which he found to be competitive in stability with its linear triplet form, has been instrumental in the closed-shell vs. open-shell debate about small carbon clusters. Cyclic forms of C_5 and C_6 have been observed spectroscopically, while reports of rhombic C_4 have been reported in Coulomb explosion experiments.
- NMR coupling constants His EOM-CCSD work was the first to offer predictive results for NMR coupling constants whose average errors are ~ 3Hz. With this tool, he provided fingerprints for the non-classical bridged H atom in ethylcarbenium and the bridged, pentacoordinate C atom in the 2-norbornyl cation which had resisted experimental determination. The observed coupling constants are also in exceptional agreement with those that could be obtained experimentally by Olah, substantiating the accuracy of his predictions. For H bonds he provides formulae to relate the two-bond coupling constant to the distance between the atoms that are H-bonded which provides a new probe to assist biomolecular structure determination that is complementary to X-ray determination where the H atoms cannot be observed.

His group continually introduces new correlated quantum chemical methods:

- EOM-CC and STEOM-CC for excited, ionized, and electron attached states for molecules, recently generalizing the former to the full EOM-CCSDT. Like the CC methods for ground states, these methods offer the same unambiguous application to excited states, with similar successes.
- New correlated methods for polymers, recently reporting the first CCSD results

- *Ab Initio* density functional theory, an approach that unlike other current hybrid or gradient corrected DFT methods has to converge to the right answer in the limit like *ab initio* quantum chemistry. The most recent work derives the exact exchange-correlation potential of DFT from coupled-cluster theory, making a seamless connection between wave-function theory and density functional theory.
- The 'transfer Hamiltonian' procedure to make it possible to do quantum mechanically based, 'predictive' simulations for materials.
- The natural linear scaled coupled-cluster method (NLSCC) which unlike others, makes it possible to use large basis sets in the quasi-separable units based upon natural bond localized orbitals. It also has the advantage that it only uses orthogonal unoccupied molecular orbitals which has significant computational advantages over projected atomic orbital methods. NLSCC also provides transferable cluster amplitudes that reflect conventional chemical intuition.

SIGNIFICANT PUBLICATIONS IN THEORY AND APPLICATION

Theory

1. R. J. Bartlett and G. D. Purvis, "Many-body perturbation theory, coupled-pair many-electron theory and the importance of quadruple excitations for the correlation problem," Proceedings of the American Theoretical Chemistry Conference, Boulder, Colorado, Int. J. Quantum Chem. **14**, 561-581 (1978).
2. R. J. Bartlett and G. D. Purvis III, "Molecular applications of coupled cluster and many-body perturbation methods," Proceedings of the Nobel Symposium on Many-Body Theory, Lerum, Sweden, Physica Scripta **21**, 255-265 (1980).
3. G. D. Purvis, III and R. J. Bartlett, "A full coupled-cluster singles and doubles model: The inclusion of disconnected triples," J. Chem. Phys. **76**, 1910-1918 (1982).
4. L. Adamowicz, W. D. Laidig and R. J. Bartlett, "Analytical gradients for the coupled-cluster method," Int. J. Quantum Chem. Symp. **18**, 245-254 (1984).
5. Y. S. Lee, S. A. Kucharski and R. J. Bartlett, "A coupled cluster approach with triple excitations," J. Chem. Phys. **81**, 5906-5912 (1984).
6. J. Noga and R. J. Bartlett, "The full CCSDT model for molecular electronic structure," J. Chem. Phys. **86**, 7041-7050 (1987).
7. R. J. Bartlett, "Coupled-cluster approach to molecular structure and spectra: A step toward predictive quantum chemistry," J. Phys. Chem. (Feature Article) **93**, 1697-1708 (1989).

8. S. A. Kucharski and R. J. Bartlett, “The coupled-cluster single, double, triple and quadruple excitation method,” J. Chem. Phys. **97**, 4282-4288 (1992).
9. J. F. Stanton and R. J. Bartlett, “The equation of motion coupled-cluster method. A systematic biorthogonal approach to molecular excitation energies, transition probabilities, and excited state properties,” J. Chem. Phys. **98**, 7029-7039 (1993).
10. M. Nooijen and R. J. Bartlett, “A new method for excited states: Similarity transformed equation-of-motion coupled-cluster theory,” J. Chem. Phys. **106**, 6441-6448 (1997).
11. N. Flocke and R.J. Bartlett, “A natural linear scaling coupled-cluster method,” J. Chem. Phys. **121**, 10935 (2004).
12. R. J. Bartlett, V. F. Lotrich, I.V. Schweigert, “*Ab initio* DFT: The best of both worlds?” J. Chem. Phys. **123**, 062205 (2005).
13. A. Taube and R.J. Bartlett, “Frozen natural orbital coupled-cluster theory: Forces and applications to decomposition of nitroethane,” J. Chem. Phys. **128**, 164101/1 – 164101/17 (2008).
14. R. J. Bartlett, “Towards an exact correlated orbital theory for electrons,” Frontiers Article, Chem. Phys. Lett. **484**, 1-9 (2009).
15. M. Musial, A. Perera, and R.J. Bartlett, “Multireference coupled-cluster theory: The easy way,” J. Chem. Phys. **134**, 114108/1-10 (2011).
16. P. Verma and R.J. Bartlett, “Increasing the applicability of density functional theory. III. Do consistent Kohn-Sham density functional methods exist?” J. Chem. Phys. **137**, 134102/1-12 (2012).
17. T.J. Watson, Jr., V. Lotrich, P. Szalay, A. Perera, and R.J. Bartlett, “Benchmarking for perturbative triple-excitations in EE-EOM-CC methods,” J. Phys. Chem. A **117**, 2569-2579 (2013).

Applications

1. R.J. Bartlett, I. Shavitt and G.D. Purvis III, "The quartic force field of H_2O determined by many-body methods that include quadruple excitation effects,” J. Chem. Phys. **71**, 281-291 (1979).
2. D. H. Magers, R. J. Harrison and R. J. Bartlett, “Isomers and excitation energies of C_4,” J. Chem. Phys. **84**, 3284-3290 (1986).
3. J. F. Stanton, W. N. Lipscomb and R. J. Bartlett, “Structure, energetics and vibrational spectra of beryllium borohydride isomers,” J. Chem. Phys. **88**, 5726-5734 (1988).

4. W. J. Lauderdale, J. F. Stanton and R. J. Bartlett, “Stability and energetics of metastable molecules: tetraazatetrahedrane (N_4), hexaazabenzene (N_6), and octaazacubane (N_8),” J. Phys. Chem. **96**, 1173-1178 (1992).
5. J. D. Watts and R. J. Bartlett, “A theoretical study of linear carbon cluster monoanions, C_n^- and dianions, C_n^{2-} (n = 2–10),” J. Chem. Phys. **97**, 3445-3457 (1992).
6. K.F. Ferris and R.J. Bartlett, " Hydrogen pentazole: does it exist?" J. Am. Chem. Soc. (Communication) **114**, 8302-8303 (1992).
7. H. Sekino and R. J. Bartlett, “Molecular hyperpolarizabilities,” J. Chem. Phys. **98**, 3022-3037 (1993).
8. S. A. Perera, R. J. Bartlett and P. von R. Schleyer, “Predicted NMR coupling constants and spectra for ethyl carbocation: A fingerprint for nonclassical hydrogen-bridged structures,” J. Am. Chem. Soc. (Communication) **117**, 8476-8477 (1995).
9. J. Q. Sun and R. J. Bartlett, “Correlated prediction of the photoelectron spectrum of polyethylene: explanation of XPS and UPS measurements,” Phys. Rev. Lett. **77**, 3669-3672 (1996).
10. A. Perera and R.J. Bartlett, "Structure and NMR spectra of the 2-norbornyl carbocation: prediction of $^1J(^{13}C^{13}C)$ for the bridged, pentacoordinate carbon atom," J. Am. Chem. Soc. (Communication). **118**, 7848-7850 (1996).
11. P. B. Rozyczko, S. A. Perera, M. Nooijen, and R. J. Bartlett, “Correlated calculations of molecular dynamic polarizabilities,” J. Chem. Phys. **107**, 6736-6747 (1997).
12. A. Perera and R.J. Bartlett, " NMR spin-spin coupling constants for hydrogen bonds of $[F(HF)_n]^-$, n=1-4, clusters," J. Am. Chem. Soc. (Communication). **122**, 1231-1232 (2000).
13. J. E. Del Bene, S. A. Perera, and R. J. Bartlett, "^{15}N-^{15}N spin coupling constants across N-H-N and N-H+-N hydrogen bonds: Can coupling constants provide reliable estimates of N-N distances in biomolecules?" Mag. Res. In Chem. **39**, S109-S1114 (2001).
14. T. Kus, V.F. Lotrich, A. Perera, and R. J. Bartlett, “An *ab initio* study of the $(H_2O)_{20}H^+$ and $(H_2O)_{21}H^+$ water clusters,” J. Chem. Phys. **131**, 104313/1 – 104313/6 (2009).
15. R. Molt, Jr., T. Watson, Jr., V.F. Lotrich, and R.J. Bartlett, “RDX geometries, excited states, and revised energy ordering of conformers via MP2 and CCSD(T) methodologies: Insights into decomposition mechanism,” J. Phys. Chem. A **115**, 884-890 (2011).

16. P.G. Szalay, T. Watson, A. Perera, V. Lotrich, and R.J. Bartlett, “Benchmark studies on the building blocks of DNA. 3. Watson-Crick and stacked base pairs,” J. Phys. Chem. A **117** (15), 3149-3157 (2013).

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EDUCATION

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Millsaps College, B.S. 1966 Chemistry and Mathematics (double major)

University of Florida, PhD 1971, Quantum Chemistry

ACADEMIC POSITIONS

INDEX TOP

Graduate Research Professor, University of Florida, 1988–present

Professor of Chemistry and Physics, University of Florida, 1981–1987

Guggenheim Fellow, Harvard University, University of California at Berkeley, 1986–1987

Visiting Scientist, Max Planck Institut für Astrophysik, Garching bei München, Germany, 1983

Adjunct Assistant Professor, Washington State University, 1975–1977

Associate Research Scientist, The Johns Hopkins University, 1972–1974

NSF Postdoctoral Fellow, Aarhus University, Denmark, 1971–1972

IBM Predoctoral Fellow, University of Florida, 1969–1971

NDEA Title IV Predoctoral Fellow, University of Florida, 1966–1969

HONORS & AWARDS

INDEX TOP

The American Chemical Society (ACS) award in Theoretical Chemistry (2007)

The Schrödinger Medal of the World Association of Theoretical and Computational Chemists (WATOC) (2008)

The Boys-Rahman Prize of the Royal Society of Chemistry (RSC) (2009)

The Southern Chemist of the Year (2010), Memphis section of the ACS

Humboldt Research Award (2014)

Honoree, 7th Molecular Quantum Mechanics – Electron Correlation: The Many-Body Problem at the Heart of Chemistry, an International Conference in honor of Rodney J. Bartlett, Lugano, Switzerland, June 2013

The Florida ACS Award (2000)

Doctor Honoris Causa, Comenius University, Bratislava, Slovakia October, 2012

Doctor of Science, Honoris Causa, Millsaps College, April, 2011

Symposium in honor of RJB, 235th American Chemical Society National Meeting, New Orleans, LA, April 2008

FELLOWSHIPS

INDEX TOP

Fellow, International Academy of Quantum Molecular Sciences, 1991; Bureau 2006

Fellow, American Chemical Society Fellow, 2010

Fellow, American Physical Society, 1989

Fellow, Guggenheim Foundation, 1986

E.T.S. Walton Fellow, Science Foundation Ireland, University College Cork, Cork, Ireland, 2003

SPECIALLY INVITED LECTURESHIPS

INDEX TOP

November 2013 – Lise Meitner Lecturer, Weisman Institute of Science, Rehovoth, Israel

January 2013 – Davidson Lecturer, University of North Texas, Denton, TX

November 2010 – Pitzer Lecturer in Theoretical Chemistry, Ohio State University, Columbus, OH

May 2010 – S.F. Boys – A. Rahman Award Lecture Series, University of Nottingham, Nottingham, England, University of Manchester, Manchester, England, and Heriot-Watt University, Edinburgh, Scotland

June 2009 – Löwdin Lecture, Uppsala Universitet, Uppsala, Sweden

September 2008 – Eighth Triennial Congress of the World Association of Theoretical and Computational Chemistry (WATOC), Sydney, Australia upon receiving the Schrödinger Medal

December 2007 – "Coupled-Cluster Theory in Quantum Chemistry: The Emergence of a New Paradigm," THE BARTLETT LECTURE, 16th Conference on Current Trends in Computational Chemistry, Jackson, MS (The honoree gives a lecture named for him/herself.)

July 2007 – CRANN Distinguished Lecturer, Trinity College, Dublin, Ireland

March 2007 – 3rd Annual Löwdin Lecture, University of Florida, Gainesville, FL

March 2007 – "Coupled-cluster Theory in Quantum Chemistry: The Emergence of a New Paradigm," AWARDS SYMPOSIUM, National ACS Meeting, Chicago, IL, upon receiving the ACS Award in Theoretical Chemistry

January 2007 – Coochbehar Professorship Lecture, Indian Association for the Cultivation of Science, Kolkata, India

November 2006 – The 1st Roger E. Miller Lecture, University of Waterloo, Waterloo, Canada

June 2004 – Professeur Invité ULP, Université Louis Pasteur, Strasbourg, France

June 2001 – Second Kapuy Memorial Lecture, Budapest, Hungary.

February 2000 - Bircher Lecture, Vanderbilt University, Nashville, TN

April 1999 - Distinguished Lecture Series in Computational Chemistry and Physics at Jackson State University, Jackson, MS

October 1995 – Korean Lecture Series: Advanced Institute of Science and Technology, Taejon, Korea; Postec University, Pohang, Korea; Kangnung National University, Kangnung, S. Korea.

May 1993 - 11th Robert S. Mulliken Lecturer, University of Georgia, Athens, GA

March 1987 - Distinguished Lecturer, University of Arkansas.

EDITORIAL POSITIONS

INDEX TOP

Editorial Board, Molecular Physics, 1999-present

Board, Molecular Physics, 1992-1998

Editorial Board, Journal of Chemical Physics, 1990–1992

Advisory Board, Theoretica Chimica Acta, 1987–1997

Theoretical Chemistry Accounts, 1997– present

Editorial Board, International Journal of Quantum Chemistry, 1985–1989

OTHER ACADEMIC AFFILIATIONS

INDEX TOP

Chairman, Subdivision of Theoretical Chemistry, ACS, 1985

Chairman-Elect, Subdivision of Theoretical Chemistry, ACS, 1984

NONACADEMIC POSITIONS

INDEX TOP

Group Leader, Chemical Physics, Battelle Memorial Institute, 1979–1981

Senior Research Scientist, Battelle Memorial Institute, 1977–1979

Senior Research Scientist, Battelle Pacific Northwest Laboratory, 1976–1977

Principal Research Scientist, Battelle Pacific Northwest Laboratory 1974–1976

CONSULTATION OUTSIDE UNIVERSITY OF FLORIDA

INDEX TOP

Advisory Board, Institute for Advanced Study, Massey University, Auckland, New Zealand, (2007 -)

Advisory Board, Tyndall Research Institute, Cork, Ireland (2006 -)

Advisory Board, College of Science Engineering and Technology, Jackson State University, Jackson, MS (2006 -)

National Science Foundation, Small Business Innovation Research Program, Peer Review Panel, September 1997

Advisory Board, Maui High Performance Computing Center (1995–)

Advisory Board, Battelle, Pacific Northwest Laboratory's Molecular Center (1986–1988).

Senior Affiliate Scientist, Pacific Northwest Laboratory (1989–1992).

External Examiner for Doctor of Science Degree, Åarhus University, Åarhus, Denmark

External Examiner for PhD, Guelph-Waterloo Graduate Center, Guelph, Ontario, Canada

INVITED LECTURES AT PROFESSIONAL CONFERENCES INDEX TOP

July 2016 – International Society for Theoretical Chemical Physics (ISTCP-IX), Grand Forks, ND

June 2-16 – Molecular Quantum Mechanics (MQM) VIII, Uppsala, Sweden

Feb 2016 – Workshop Honoring Peter Schwerdtferger's 60th Birthday, Center for Theoretical Chemistry and Physics, New Zealand Institute for Advanced Study, Albany New Zealand

Dec 2015 – 2015 International Chemical Congress of Pacific Basin Societies (Pacifichem), Honolulu, HI

Nov 2015 – 67th Southeastern and 71st Southwestern Regional Meeting of the American Chemical Society, Memphis, TN

May 2015 – Frontiers in Electronic Structure Theory, a meeting in honor of Sourav Pal's 60th Birthday, Goa, India

May 2015 - Air Force Office of Scientific Research Contractors Meeting, Albuquerque, NM

May 2015 – HASI Kick-off/Frontier Project Review, Vicksburg, MS

May 2014 – FAME (Florida Annual Meeting & Exhibitions) 2013, Computational Chemistry Symposium, Tampa, FL

October 2014 – 10th Triennial Congress of World Association of Theoretical and Computational Chemists (WATOC), Santiago, Chile

March 2014 – 25th Austin Symposium on Molecular Structure and Dynamics, Dallas, TX

September 2013 – 246th National Meeting of the American Chemical Society, "Quantum Mechanics in Many Dimensions: New Challenges and Solutions for Chemical Theory," Indianapolis, IN

September 2013 - Frontiers of Theoretical Chemistry–the Parr Celebration, Duke University, Durham, NC

August 2013 – VIIIth Congress of the International Society of Theoretical Chemical Physics, Budapest, Hungary

May 2013 – FAME (Florida Annual Meeting & Exhibitions) 2013, Computational Chemistry Symposium, Tampa, FL

November 2012 – 21st Conference on Current Trends in Computational Chemistry, Jackson, MS

October 2013 – Special Symposium in honor of Prof. Miroslav Urban and Ivan Hubač, J. Heyrovsky Institute of Physical Chemistry, Comenius University, Bratislava, Slovakia

September 2012 – 3rd Conference on Theory and Applications of Computational Chemistry, Pavia, Italy

June 2012 – 3rd International Symposium and Workshop on Electron Correlations and Materials Properties of Compounds and Alloys, Porto Heli, Greece

June 2012 – Coupled-Cluster Theory and Related Methods, a satellite meeting of the 2012 International Congress of Quantum Chemistry, Boulder, CO

May 2012 - Air Force Office of Scientific Research Contractors Meeting, Washington, DC

May 2012 – South Eastern Theoretical Chemistry Association Annual Meeting, Athens, GA

January 2012 – Summer Talks in Santiago. III. Recent Developments in Quantum Chemistry (in honor of Prof. Peter Politzer), Santiago, Chile

December 2011 – 5th Asian Pacific Conference of Theoretical and Computational Chemistry, Rotorua, New Zealand

September 2011 – 10th Central European Symposium on Theoretical Chemistry (CESTC 2011), Torun, Poland

September 2011 – “Looking at the world from a coupled-cluster perspective,” 7th Congress of the International Society for Theoretical Chemical Physics, Tokyo, Japan

August 2011 – “Different approaches to the correlation problem,” American Chemical Society 242nd National Meeting, Denver, CO

July 2011 - "Strongly correlated systems, cooperativity and valence-bond theory," Workshop on Strongly Correlated Systems, Cooperativity And Valence-Bond Theory, A Coruña, Spain

July 2011 – “Multi-reference coupled-cluster theory: The easy way,” WATOC 2011, Santiago de Compostela, Spain

December 2010 – “Different Approaches to Excited States and Multi-Reference Problems,” Pacifichem Meeting 2010, Honolulu, HI

December 2010 – Computational/Experimental Characterization of Advanced Materials, SE/SW Regional ACS Symposia, New Orleans, LA

October 2010 – "The Coupled-Cluster Revolution," Symposium in Honor of Jiří Čížek and Joef Paldus, 8th International Conference of Computational Methods in Science and Engineering, Kos, Greece

September 2010 – "Do we really need DFT? Alternative correlated orbital theories from wavefunction theory," Celebrating Computational Biology: A Tribute to Frank Blaney, Oxford, England

June 2010 – "RPA: The Viewpoint of Coupled-Cluster Theory and Some Consequences," CECAM Conference on Van der Waals Forces in DFT, RPA and Beyond, Lausanne, Switzerland

November 2009 – Conference on the Occasion of Lipscomb's 90th Birthday, Boston, MA

July 2009 – Canandian Conference on Computational Chemistry VII, Halifax, Nova Scotia

May 2009 – Air Force Office of Scientific Research Contractors Meeting, San Diego, CA

March 2009 – American Chemical Society Spring 2009 National Meeting, Salt Lake City, UT

March 2009 – Horiba International Conference on Simulations and Dynamics for Nanoscale and Biological Systems, University of Tokyo, Tokyo, Japan

December 2008 – Celebration of Forty Years of Theoretical Chemistry at Aarhus University, Aarhus, Denmark

September 2008 - Eighth Triennial Congress of the World Association of Theoretical and Computational Chemistry (WATOC), Sydney, Australia

July 2008 – Symposium on "50 Years of Coupled Cluster Theory," Institute of Nuclear Theory, University of Washington, Seattle, WA

July 2008 - Sixth Congress of the International Society for Theoretical Chemical Physics, Vancouver, Canada

June 2008 – "Ab initio DFT: The seamless connection with wave-function theory," UNEDF SciDAC Annual Workshop Pack Forest, WA

September 2007 – Local Correlation Methods: From Molecules to Crystals (LCC2007), Dresden, Germany

September 2007 – Symposium on Advanced Methods of Quantum Chemistry Physics, Toruń, Poland

May 2007- "Is there something better than ccsd(t) for molecular applications? Molecular Quantum Mechanics Analytic Gradients and Beyond, A meeting in honor of Peter Pulay, Budapest, Hungary

March 2007 **-** "Coupled-cluster theory: the emergence of a new paradigm" AWARDS SYMPOSIUM, National ACS Meeting, Chicago, IL

January 2007 – “Coupled-Cluster Theory for Large Molecules: The Natural Linear Scaled Coupled-Cluster Method,” Recent Trends in Many-Body Methods for Electronic Structure and Properties of Atoms and Molecules, Bhubaneshwar (Orissa), India

January 2007 – “Natural Linear Scaling Coupled-Cluster Method and Some Other Advances for Large Calculations,” NW Chem Meeting on Science Driven Petascale Computing and Capability Development at EMSL, Richland, WA

December 2006 – LLNL International Workshop on Correlated Electrons in Matter, Half Moon Bay, CA

October 2006 - “Coupled-Cluster Theory for Large Molecules: The Natural Linear Scaled Coupled-Cluster Method,” Vedene Smith Memorial Symposium, International Conference of Computational Methods in Sciences and Engineering, Crete, Greece

October 2006 - “Coupled-Cluster Theory for Large Molecules: The Natural Linear Scaled Coupled-Cluster Method,” Symposium on Chemical Physics, University of Waterloo, Waterloo, Canada

September 2006 - Air Force Office of Scientific Research Polynitrogen Workshop at University of California, Los Angeles, CA

July 2006 – “Progress in Ab Initio DFT,” 6th Canadian Computational Chemistry Conference, Vancouver, Canada

June 2006 – “Linear Scaling,” AFOSR Annual Review Meeting, Washington, DC

May 2006 – “Addition by Subtraction in Coupled-Cluster Theory: The nCC Hierarchy,” Canadian Society for Chemistry, Halifax, Nova Scotia

May 2006 – “Addition by Subtraction in Coupled-Theory: A Reconsideration of the Coupled-Cluster/CI Interface,” Chemical Accuracy and Beyond, Satellite Meeting of the XIIth Congress of the International Academy of Quantum Molecular Sciences, Tokyo, Japan

March 2006 – “Ab Initio Density Functional Theory: The Seamless Connection with Wavefunction Theory,” ACS Meeting in Honor of Robert G. Parr, Atlanta, GA

October 2005 – “Electronic Structure of Molecules and Materials: From Coupled-Cluster Theory to DFT to the Transfer Hamiltonian,” International Conference of Computational Methods in Sciences and Engineering, Loutraki, Greece

September 2005 – “Addition by Subtraction in Coupled-cluster Theory: A reconsideration of the Coupled-cluster/CI Interface,” 13th European Seminar on Computational Molecular Quantum Chemistry Conference, Smolenice, Slovakia

September 2005 – “Progress and Problems in ab initio DFT for Ground and Excited States,” 11th International Conference on the Applications of Density Functional Theory in Chemistry and Physics, Geneva, Switzerland

August 2005 – “Energy Landscapes and Advances in Coupled-Cluster Theory,” Fall ACS 230th National Meeting, Washington, DC

August 2005 – “Progress and Problems in ab initio DFT for Ground and Excited States,” Structure and Function of Chemistry and Biology: Celebrating Prof. William Lipscomb’s 85th Birthday, Shanghai, China

July 2005 – Fifth Congress of the International Society of Theoretical Chemical Physics, New Orleans, LA

June 2005 – “Weak Interactions in DFT: The Right Answer for the Right Reasons,” CECAM Workshop on Van der Waals Forces and Density Functional Theory, Lyon France

March 2005 – J. Pople Memorial Symposium, ACS 229th Spring National Meeting, San Diego, CA

January 2005 – Computational Tools for Molecules, Clusters, and Nanostructures: A Meeting in Honor of Reinhardt Ahlrichs, Karlsruhe, Germany

January 2005 – Fifth Congress of the World Association of Theoretically Oriented Chemists, Cape Town, South Africa

December 2004 – Consortial Workshop on Computational Physics 2004, Hsinchu, Taipei, Taiwan

October 2004 – 2004 Army Energetic Materials MURI and DURINT Reviews, Picatinny, NJ

September 2004 – Electronic Structure: Principles and Applications (ESPA-2004), Valladolid, Spain

June 2004 –NSF Division of Materials Research ITR Computational Workshop, HEDM, Champaign, IL

June 2004 – Nano Principal Investigators Meeting, DARPA, Arlington, VA

May 2004 – “Some Considerations of Response Functions, Excited States, and Triple Excitations,” Response Theory and Molecular Properties, Sandbjerg Manor, Sonderborg, Denmark

May 2004 – AFOSR Molecular Dynamics Contractors Meeting, Newport, RI

Feb 2004 – Correlated Orbital Theories (On DFT and WFT: The Development of an Exact One-particle Theory for Molecules), Theory and Applications of Computational Chemistry, Gyeongji, Korea

December 2003 – “Atomic Scale Materials Design: Modeling & Simulation” Materials Research Society, Boston, MA

October 2003 – “*Ab initio* Predictions of PES for Chemical Reactions,” Review of Energetic Materials DURINT and MURI Programs, Aberdeen, MD

September 2003 – “Metastable Molecules in Ground and Excited States,” 2nd Advanced Energetics Technical Exchange, Aberdeen, MD

September 2003 – “Coupled-cluster Methods and Their Applications to Energetic Molecules,” 226th ACS National Meeting, New York, NY

August 2003 – "High Level Couple Cluster Theory: What Did We Learn?" 8th European Conference on Quantum Systems in Chemistry and Physics, Spetses, Greece

July 2003 – "*Ab Initio* Density Functional Theory," Electron Correlation: *Ab initio* Methods and Density Functional Theory, Satellite Meeting of the XIth International Congress of Quantum Chemistry, Bad Herrenalb, Germany

April 2003 – "Frontiers in Theoretical Chemistry," a Symposium in Honor of Prof. Rudolph A. Marcus, Los Angeles, CA

March 2003 – "From Wave Function Theory to Density-Functional Theory and Back," 225th ACS National Meeting, New Orleans, LA

October 2002 – "Scalable Software for Computational Chemistry," University of Kentucky, Lexington, KY

October 2002 – "*Ab initio* Predictions of PES for Chemical Reactions," MURI Kick-off Meeting, Aberdeen, MD

September 2002 – "Large Scale Dynamics with Quantum Mechanical Forces," Symposium and Summer School on Nano and Giga Challenges in Microelectronics Research and Opportunities, Moscow, Russia

September 2002 – "Predictive Theory from Molecules to Materials," Science at the Edge, Michigan State University, East Lansing, MI

July 2002 – "Advances in Electronic Structure Theory: Current Trends and Future Prospects," ICTCP-IV, Marly-le-Roi, France

June 2002 – "Predictive Theory from Molecules to Materials," Symposium to Initiate Joint Ph.D. Program between France and the United States, Strasbourg, France

June 2002 – "Large Scale Simulations with Quantum-Mechanical Forces," European Materials Research Society Spring Meeting, Strasbourg, France

June 2002 – "The Exchange Correlation Potential in *ab initio* DFT: What Does the 'Right' Exchange Correlation Allow Us to Do?" CECAM Workshop, Lyon, France

April 2002 – "Speculation on High Nitrogen Molecules," BMAED Committee on Advanced Energetic Materials and Manufacturing Technologies, Washington, DC

April 2002 – "Advances in the Treatment of Electron Correlation in Molecules: Coupled-Cluster Theory and *ab initio* DFT," 223rd ACS National Meeting, Orlando, FL

March 2002 – "Large Scale Simulations with Quantum Mechanical Forces," March APS Meeting 2002, Indianapolis, IN

January 2002 – "Predictive Theory from Molecules to Materials," University of Tennessee Chemicals Physics Workshop, Knoxville, TN

October 2001 – "Modern Aspects of Many-Electron-Theory," WE-Heraeus-Seminar, Bad Honnef, Germany

September 2001 – "Ab Initio DFT," WOG – Density Functional Theory, Brussels, Belgium

September 2001 – “Ab Initio DFT,” 9th International Conference on the Applications of the Density Functional Theory in Chemistry and Physics, San Lorenzo de El Escorial, Madrid, Spain.

September 2001 – “NMR Coupling Constants Across H-Bonds,” The Role of Predictive Theory, Strasbourg, France

September 2001 – “NMR Coupling Constants Across H-Bonds,” The Role of Predictive Theory, Torun University, Poland

September 2001 – "Ab Initio DFT," Austrian – Czech – Polish – Slovak Symposium on Quantum Chemistry, Ustron-Jaszowiec, Poland

August 2001 – “Polynitrogen molecules that don’t exist that should,” DARPA HEDM/NANO Workshop, Rosslyn, VA

July 2001 - "Ab Initio Density Functional Theory," Molecular Quantum Mechanics: The Right Answer for the Right Reason, An International Conference in Honor of Professor Ernest R. Davidson, Seattle, WA

June 2001 - "Electron correlation in Molecules and Polymers: From Coupled-Cluster theory to Ab Initio DFT," The 2nd International Workshop on Electron Correlations and Materials Properties, Rhodes, Greece

May 2001 - "Ab Initio DFT," AFOSR Molecular Dynamics/Theoretical Chemistry (MD/TC) Contractor's Meeting, Irvine, CA

December 2000 - "Ab Initio Density Functional Theory," PACIFICHEM (2000 International Chemical Congress of Pacific Basin Societies), Honolulu, HI

October 2000 - "Prospects for Polynitrogen HEDMS," DARPA Polynitrogen HEDM Program, Salt Lake City, UT

October 2000 - "New Developments in Theory and their Applications to HEDM's," 2000 Air Force High Energy Density Matter (HEDM) Contractors Conference, Salt Lake City, UT

July 2000 – "Ab Initio Density Functional Theory,” 4th Canadian Computational Chemistry Conference, Bishop’s University, Lennoxville, Québec, Canada

May 2000 – "Predicted NMR Coupling Constants Across Hydrogen-Bonds: A Fingerprint for Specifying Hydrogen Bond Type?” SETCA 2000, University of Georgia, Athens, GA

May 2000 –"Ab Initio Density Functional Theory,” Twelfth Annual Workshop on Recent Developments in Electronic Structure Methods,” Georgia Institute of Technology, Atlanta, GA

May 2000 - "Predicted NMR Coupling Constants Across Hydrogen-Bonds: A Fingerprint for Specifying Hydrogen Bond Type,?" Morley Award Symposium for Isaiah Shavitt, Cleveland, OH

May 2000 – “Fingerprint for Specifying Hydrogen Bond Type?" Lipscomb Festschrift, Harvard University, Cambridge, MA

May 2000 - " Predicted NMR Coupling Constants Across Hydrogen-Bonds: A Fingerprint for Specifying Hydrogen Bond Type?" FAME 2000, Orlando, FL (presented when receiving the Florida Award)

April 2000 – "Ab Initio Density Functional Theory," Fifth European Workshop on Quantum Systems in Chemistry and Physics, Uppsala, Sweden, April 13-18 2000

February 2000 - "Ab Initio Density Functional Theory," 40th Sanibel Symposium, St. Augustine, FL

January 2000 –"High Energy Density Materials," HEDM/DARPA Meeting, Arlington, VA

November 1999 - "Correlation in Molecules and Solids," The Third Congress of the International Society for Theoretical Chemical Physics, Mexico City, Mexico

October 1999 - "Excited States in Molecules and Solids Interplay between Experiment and Theory," ESMS 99 Conference, Tarragona, Spain

September 1999 - "Computational Methods in Quantum Chemistry," 11th Strasburg Seminar on Computational Methods in Quantum Theory, Zakopane, Poland

August 1999 - "On the Interface of Density Functional Theory with Correlated Ab Initio Methods," American Chemical Society National Meeting, New Orleans, LA

August 1999 - "Nonlinear Optics," American Chemical Society National Meeting, New Orleans, LA, August 23-27, 1999.June 1999 - "N_2O Dimers, Trimers and Tetramers: A New Class of Potential HEDM's," Air Force Office of Scientific Research Annual Contractor's Review, Cocoa Beach, FL

June 1999 - "A Survey of Polynitrogen Systems: N_2-N_8 ," DARPA Meeting, Cocoa Beach, FL, June 11, 1999.March 1999 - "Coupled-Cluster Theory, Density Functional Theory, and Excited States," American Physical Society Centennial Meeting, Atlanta, GA

January 1999 - Meeting of High Energy Density Materials research group at US Air Force, Arlington, VA

October 1998 - "Response Theory in Density Functional Theory and Coupled-Cluster Theory," CECAM (European Centre for Atomic and Molecular Computations) Workshop on Electronic Response Functions in Atoms, Molecules, and Solids, Lyon, France, October 5-7, 1998

September 1998 - "The Coupled-Cluster Treatment of NMR and ESR Spectra," International Conference on Quantum Chemical Calculations of NMR and EPR Parameters, Bratislava-Smolenice, Slovak Republic, September 14-18, 1998.

August 1998 - "Twenty Years of Coupled-cluster Theory: Overview and Reflection," Physical Chemistry Division symposium, *A Celebration of 20 Years of the Subdivision of Theoretical Chemistry*, American Chemical Society National Meeting, Boston MA, 23-27 August 1998.

May 1998 - "Quantum Chemistry at the Interface of Density Functional Theory and *ab initio* Correlated Methods," 27th Annual Meeting of the Southeastern Theoretical Chemistry Association, The Florida State University, Tallahassee FL

May 1998 - “Does the O_4 Molecule Exist?” 1998 High Energy Density Matter Contractor’s Meeting, AFOSR, Monterey CA

January 1998 - “The Potential Role of Excited States and Electron-attached States in the Initial Steps of Detonation,” Energetic Materials Workshop, ONR, Annapolis MD.

September 1997 - “The Equation-of-Motion Coupled-Cluster Method and Its Similarity-Transformed (STEOM) Variant, as a Unified Treatment of Excited, Ionized, Electron-Attached States and Properties,” International Conference on Electron Correlation: From Atoms to Biomolecules; Glumslov, Sweden.

June 1997 - “New Methods for Excited States,” 1997 High Energy Density Matter Contractor’s Meeting, U.S. Air Force Office of Scientific Research, Chantilly, VA.

June 1997 - “The Interface Between DFT and *ab initio* Correlated Methods,” Symposium on Density Functional Theory and Applications, Duke University, Durham, North Carolina

February 1997 - “Non-linear Optical Properties of Molecules: The Role of Quantum Chemistry,” Wright Patterson Air Force Base, Dayton, OH.

February 1997 - “Electron Correlation in Extended Systems: The Next Frontier?” Ohio Supercomputer Center, Columbus, OH

December 1996 - “Energetic Materials Workshop,” Office of Naval Research, Washington, DC

October 1996 - “Electron Correlation in Polymers,” Swedish-American Symposium on the Foundations of Quantum Theory in Chemistry, Molecular Physics and Biology: A Symposium in Honor of Per-Olöv Löwdin,” Sanibel, FL.

August 1996 - Battelle Northwest Laboratories, EMSL Theory, Modeling and Simulation Workshop, “Recent Developments in Coupled-Cluster Theory Implemented into the ACES II Program System,” Richland, Washington

July 1996 - “The First Principle Prediction of Coupling Constants for Carbocations and Other Molecules,” World Association of Theoretically Oriented Chemists (WATOC) Congress, Jerusalem, Israel

April 1996 - “NMR Coupling Constants with the Equation-of-Motion Coupled-Cluster Method,” 2nd International Congress on Theoretical Chemical Physics, New Orleans, LA

March 1996 - “Perturbation Approaches for Excited States,” Research Symposium on Multiconfigurational Perturbation Theory: Methods and Applications. Gandia, Spain.

December 1995 - “Challenges for HPCC,” Computational Chemistry Focus Group, Maui, Hawaii.

November 1995 - “Electronic Excited States of Organic Molecules,” Joint Regional ACS Meeting, Memphis, TN

October 1995 - “Coupled-Cluster Theory as a Unified Approach to Molecular Spectroscopy: Vibrational, Electronic, and NMR,” Korean Chemical Society, Pusan, Korea.

October 1995 - “Initial Steps to Detonation of Explosives,” ONR Workshop, Michigan Technological University, Houghton, MI.

September 1995 - “Equation-of-Motion Coupled-Cluster Method for Excited, Ionized, and Electron-Attached States,” Molecular Quantum Mechanics: Methods and Applications Conference, University of Cambridge, Cambridge, England.

August 1995 - “Excited States Using the Equation-of-Motion Coupled-Cluster Method,” 12th Canadian Symposium on Theoretical Chemistry, University of New Brunswick, Fredericton, Canada

June 1995 - “Energetic Molecules: The Role of Theory,” Office of Naval Research Data Exchange Meeting, Paris, France.

June 1995 - “Analogues of Tetrahedral N_4 as Potential High-Energy Molecules,” Air Force High Density Materials Contractors’ Conference, Woods Hole, MA.

May 1995 - “Equation-of-Motion Coupled-Cluster Methods for Excited, Ionized, and Electron-Attached States,” Pople Symposium, Northwestern University, Evanston, IL.

May 1995 - “Equation-of-Motion Coupled-Cluster Methods with Application to BCl_3,” Air Force Office of Scientific Research Contractors’ Meeting, Wright-Patterson Air Force Base, CA.

January 1995 - Air Force Office of Scientific Research HEDM Theory-Synthesis Workshop, Palmdale, CA

INVITED COLLOQUIA PRESENTED AT UNIVERSITIES AND LABORATORIES

INDEX TOP

September 2016 – Department of Chemistry, The Johns Hopkins University, Baltimore, MD

June 2016 – Center for Theoretical and Computational Chemistry, University of Oslo, Oslo, Norway

November 2013 – Technion Institute of Technology, Haifa, Israel

November 2013 – Institute of Chemistry, Hebrew University, Jerusalem, Israel

November 2013 – Lise Meitner Minerva Center for Computational Chemistry, Weisman Institute of Science, Rehovot, Israel

April 2011 - École polytechnique fédérale de Lausanne, Lausanne, Switzerland

April 2011 - Università della Svizzera italiana, Lake Lugano, Switzerland

April 2011 – Eidgenössische Technische Hochschule (Swiss Federal Institute of Technology), Zürich, Switzerland

May 2009 – University of Colorado at Boulder, Boulder, CO

April 2009 – Texas Tech University, Lubbock, TX

January 2009 – Massey University, Albany, New Zealand

July 2007 – Trinity College, Dublin, Ireland
June 2007 – Tyndall Institute, Cork, Ireland
June 2007 – Univesité Louis Pasteur, Strasbourg, France
January 2007 – National Chemical Laboratory, Pune, India
September 2005 - Comenius University, Bratislava Slovakia
July 2004 – York University, York, England
May 2004 – Universite Louis Pasteur, Strasbourg, France
July 2003 – Queens University, Belfast, Northern Ireland
June 2003 – National University of Ireland at Galway, Galway, Ireland
June 2003 – Trinity College, Dublin, Ireland
May-June 2003 – Lecture series, University College Cork, Cork, Ireland
January 2002 – University of Tennessee, Knoxville, Tennessee
September 2001 – Universite Louis Pasteur, Strasbourg, France
September 2001 – Torun University, Poland
June 2001 – Eötvos Larand University, Budapest, Hungary
April 2001 - Purdue University, West Lafayette, IN
March 2001 - UC-Berkeley, Berkeley CA
October 2000 - Virginia Tech. University, Blacksburg, VA
October 2000 - Oak Ridge National Laboratory, Oak Ridge, TN
August 2000 - University of Tennessee, Knoxville, Tennessee
December 1999 - Motorola Inc., Mesa AZ
December 1999 - Arizona State, Phoenix, AZ
September 1999 – Katowice University, Katowice, Poland
September 1999 – Torun University, Torun, Poland
January 1999 - University of Alabama, Birmingham, AL
October 1997 - Texas A&M, College Station, TX
October 1997 - University of Houston, Houston, TX
October 1997 - Rice University, Houston, TX
February 1997 - Tulane University, New Orleans, LA
December 1996 - University of Torino, Torino, Italy
April 1996 - University of North Texas, Denton, TX
April 1996 - Southern Methodist University, Dallas, TX
April 1996 - University of Texas at Arlington, Arlington, TX

October 1995 - Lehigh University, Bethlehem, PA

March 1995 - Iowa State University, Ames, IA

RESEARCH GRANTS (LAST 10 YEARS)

INDEX TOP

RJB has been the Principal Investigator on more than $8.6 million of research support over the last ten years. Grants have been received from the Air Force Office of Scientific Research, the Army Research Office, ACES QC LLC, the National Science Foundation (multi-investigator grants), the National Science Foundation International, the North Atlantic Treaty Organization, and the Office of Naval Research.

MEETINGS ORGANIZED

INDEX TOP

Co-organizer, Molecular Quantum Mechanics 2016: Uppsala, Sweden, 2016

Co-organizer, Molecular Quantum Mechanics 2013: Lake Lugano, Switzerland

Principal organizer, Sanibel Symposium, St. Simons Island, GA (annual meeting)

Principal organizer, Molecular Quantum Mechanics 2010: From Methylene to DNA and Beyond, Berkeley, CA, 2010

Principal organizer, Atomic, Chemical and Nuclear Developments in Coupled Cluster Methods Workshop, Institute for Nuclear Theory, University of Washington, Seattle, WA, June 23-July 25, 2008

Pacifichem 2005, “Theoretical Methods for Prediction of Molecular Properties,” Honolulu, Hawaii, December 15-20, 2005

Computational Materials Science Network Workshop, "Scale-Parity Multi-Scale Simulation of Chemo-Mechanical Processes," St. Augustine, FL, February, 2000 (with KDI Team)

Coupled-Cluster Theory and Electron Correlation Workshop, “*Fifty Years of the Correlation Problem*,” Cedar Key, FL, June 1997.

Symposium on “Frontiers of Electronic Structure Theory,” National ACS Meeting, San Francisco CA, April 1997 (with Martin Head-Gordon)

Principal organizer, Sanibel Symposia on the Quantum Theory of Matter, St. Augustine, FL, March 1990-1996.

Organizer of many symposia as part of Sanibel meeting, 1981-1989, 1997–present

Symposium on “Comparison of *Ab Initio* Quantum Chemistry with Experiment,” ACS National Meeting, New York City, August 1991

Symposium on “Coupled-Cluster Theory at the Interface of Atomic Physics and Quantum Chemistry,” Harvard-Smithsonian Institute for Theoretical Atomic and Molecular Physics, Cambridge, MA, August 1990.

Symposium on “Theory at the Interface of Chemistry and Biology,” National ACS Meeting, Anaheim, CA, 1986 (with H. Weinstein)

Symposium on “Comparison of *Ab Initio* Quantum Chemistry with Experiment for Small Molecules: State-of-the-Art,” National ACS Meeting, Philadelphia, PA, August 1984.

OTHER

Initiator and Director of the ACES II Workshop, 1994–present (biannual schedule, first workshop held at Ohio State University, December 1994); workshops held in Gainesville, FL; Wright Patterson Air Force Base, May, 1997.

Initiator and Director of the Florida Quantum Theory Project's Short Course on Applied Molecular Orbital Theory, 1986–1993.

PUBLICATIONS

RJB is listed at www.isihighlycited.com as one of the most cited chemists in the world. His Web of Science h-index is 96. His Google Scholar h-index is 102. His researcher ID is F-6781-2011.

I. BOOKS—EDITOR

INDEX TOP

1. Comparison of ab initio Quantum Chemistry with Experiment: State-of-the-Art, Reidel, Dordrecht, The Netherlands, 1985.
2. Recent Advances in Coupled-Cluster Methods, Volume 3 World Scientific Publishing Pte Ltd., Singapore, Republic of Singapore, 1997.
3. The Coupled Cluster Theory Electron Correlation Workshop, Fifty Years of the Correlation Program, Cedar Key, Florida, June 15-19, 1997, Mol. Phys., Vol. 94 (1998).
4. Coupled-Cluster Theory at the Interface of Atomic Physics and Quantum Chemistry, Proceedings of Workshop held at the Harvard-Smithsonian Institute for Theoretical Atomic and Molecular Physics, August 6-11, 1990, issues 2-5, Theor. Chim. Acta **80** (1990).
5. On the Occasion of Yngve Ohrn’s 60th Birthday, Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory and Computational Methods, Int. J. Quant. Chem. **28** (1994).
6. Selected Papers of Henry F. Schaefer III, (R.J. Bartlett, T.D. Crawford, M. Head-Gordon, and C.D. Sherill, editors), Brandon’s Printing, Atlanta (2010).

II. BOOKS—CONTRIBUTOR OF CHAPTER(S)

INDEX TOP

1. R. J. Bartlett and D. M. Silver, “Numerical infinite-order perturbation theory” in *Quantum Science* (J. L. Calais, O. Goscincki, J. Linderberg and Y. Öhrn, editors). Plenum, 393-408 (1976).
2. R. J. Bartlett, “Many-body perturbation theory and coupled cluster theory for electron correlation in molecules” in *Annual Reviews of Physical Chemistry*, Volume 32, 359-401 (1981).
3. G. F. Adams, G. D. Bent, R. J. Bartlett, and G. D. Purvis III, “Calculations of potential energy surfaces for HCO and HNO using many-body methods” in *Potential Energy Surfaces and Dynamics Calculations* (D. G. Truhlar, editor). Plenum, 133-167 (1981).
4. M. J. Redmon, R. J. Bartlett, B. C. Garrett, G. D. Purvis III, P. M. Saatzer, G. C. Schatz, and I. Shavitt, “Collisional excitation of H_2O by O-atom impact: Classical dynamics on an accurate *ab initio* potential energy surface” in *Potential Energy Surfaces and Dynamics Calculations* (D. G. Truhlar, editor). Plenum, 771-803 (1981).
5. R. J. Bartlett, C. E. Dykstra, and J. Paldus, “Coupled-cluster methods for molecular calculations” in *Advanced Theories and Computational Approaches to the Electronic Structure of Molecules* (C. E. Dykstra, editor). Reidel, 127-159 (1984).
6. S. A. Kucharski and R. J. Bartlett, “Fifth-order many-body perturbation and its relationship to various coupled-cluster approaches” in *Advances in Quantum Chemistry* Volume 18, 281-344 (1986).
7. N. C. Handy, R. D. Amos, J. F. Gaw, J. E. Rice, E. D. Simandrias, T. J. Lee, R. J. Harrison, W. D. Laidig, G. B. Fitzgerald and R. J. Bartlett, “Techniques used in evaluating orbital and wavefunction coefficients and property derivatives—the evaluation of M(B)P(T)-2 second derivatives” in *Geometrical Derivatives of Energy Surfaces and Molecular Properties* (P Jørgensen and J. Simons, editors). Reidel, Dordrecht, The Netherlands, 179-191 (1986).
8. R. J. Bartlett, “Analytical evaluation of gradients in coupled-cluster and many-body perturbation theory” in *Geometrical Derivatives of Energy Surfaces and Molecular Properties* (P. Jørgensen and J. Simons, editors). Reidel, Dordrecht, The Netherlands, 35-61 (1986).
9. L. Adamowicz and R. J. Bartlett, “Very accurate coupled cluster calculations for diatomic systems with numerical orbitals” in *Nobel Laureate Symposium on Applied Quantum Chemistry* (V. H. Smith, H. F. Schaefer III, and K. Morokuma, editors). Reidel, Dordrecht, The Netherlands, 111-133 (1986).
10. J. F. Stanton, R. J. Bartlett and W. N. Lipscomb, “Theoretical studies of small boranes” in *Proceedings of IMEBORON VI*. World Scientific Publishing, Singapore, 74-81 (1988).
11. J. F. Stanton, R. J. Bartlett, and W. N. Lipscomb, “A theoretical study of the unimolecular dissociation of diborane” in *Molecules in Physics, Chemistry and*

Biology, Volume III (J. Maruani, editor). Kluwer, Dordrecht, The Netherlands, 357-363 (1988).

12. R. J. Bartlett, S. A. Kucharski, J. Noga, J. D. Watts and G. W. Trucks, “Some consideration of alternative ansätze in coupled-cluster theory” in *Lecture Notes in Chemistry*, Volume 52 (U. Kaldor, editor). Springer-Verlag, Heidelberg, 125-149 (1989).

13. I. Hubac, M. Svrcek, E. A. Salter, C. Sosa and R. J. Bartlett, “Partitioning of the vibrational-electronic Hamiltonian. *Ab initio* correlated calculations of the first vibronic transitions for some simple molecules” in *Lecture Notes in Chemistry*, Volume 52 (U. Kaldor, editor). Springer-Verlag, Heidelberg, 95-124 (1989).

14. R. Mattie, M. Rittby, R. J. Bartlett, and S. Pal, “Applications of multi-reference coupled-cluster theory” in *Lecture Notes in Chemistry*, Volume 50 (D. Mukherjee, editor). Springer-Verlag, Heidelberg, 143-153 (1989).

15. S. J. Cole and R. J. Bartlett, “The electric dipole function of CO^{+}” in *Studies in Physical and Theoretical Chemistry*, Volume 62 (R. Carbo, editor). Elsevier, Amsterdam, The Netherlands, 199-211 (1989).

16. R. J. Bartlett, J. F. Stanton, and J. D. Watts, “Analytic MBPT(2) energy derivatives: A powerful tool for the interpretation and prediction of vibrational spectra for unusual molecules” in *Advances in Molecular Vibrations and Collision Dynamics*, Volume 1B (J. Bowman, editor). JAI Press, Inc., Greenwich CT, 139-167 (1991).

17. R. J. Bartlett, M. Rittby, J. D. Watts, and D. E. Bernholdt, “Carbon clusters: The synergism between theory and experiment” in *On Clusters and Clustering: From Atoms to Fractals* (P. J. Reynolds, editor). Elsevier, 23-31 (1993).

18. R. J. Bartlett and J. F. Stanton, “Applications of post-Hartree-Fock methods: A tutorial” in *Reviews in Computational Chemistry*, Volume 5 (D. Boyd and K. Lipkowitz, editors). VCH Publishers, New York, NY, 65-169 (1994).

19. R. J. Bartlett, “Coupled cluster theory: An overview of recent developments” in *Modern Electronic Structure Theory* (D. R. Yarkony, editor). World Scientific Publishing Co. Ltd., Singapore,1047-1131 (1995).

20. H. Sekino and R. J. Bartlett, “Sum-over-state representation on non-linear response properties in time dependent Hartree-Fock theory: The role of state truncation” in *Nonlinear Optical Materials* (S. Karna, editor). American Chemical Society (1996).

21. R. J. Bartlett and H. Sekino, “Can quantum chemistry provide reliable hyperpolarizabilities?” in *Nonlinear Optical Materials* (S. Karna, editor). American Chemical Society, 23-57 (1996).

22. R. J. Bartlett and J. D. Watts, “ACES II,” in *Encyclopedia of Computational Chemistry*, John Wiley & Sons, Ltd., (1999).

23. J. Sun and R. J. Bartlett, “Modern Correlation Theories for Extended, Periodic Systems” in *Topics in Current Chemistry*, Volume 203. Springer Verlag Berlin Heidelberg, 121-145 (1999).

24. D. E. Bernholdt and R. J. Bartlett, "A Critical Assessment of Multireference Fock Space CCSD and Perturbative Third-order Triples Approximations for Photoelectron Spectra and Quasidegenerate Potential Energy Surfaces" in *Advances in Quantum Chemistry,* Volume 34. Academic Press, 271-293 (1999).

25. P. Piecuch and R. J. Bartlett, "EOMXCC: A New Coupled-cluster Method for Electronic Excited States" in *Advances in Quantum Chemistry*, Volume 34. Academic Press, 295-380 (1999).

26. H. Sekino and R. J. Bartlett, "On the Extensivity Problem in Coupled Cluster Property Evaluation" in *Advances in Quantum Chemistry*, Volume 35. Academic Press, 149-173 (1999).

27. R. J. Bartlett, “Quantum Chemistry in the New Millenium: The Next Step” in *Chemistry for the 21st Century* (E. Keinan and I. Schechter, editors). Wiley-VCH, Weinheim, 271-286 (2001).

28. R.J. Bartlett, J. E. Del Bene and S.A. Perera, “Does the Magnitude of NMR Coupling Constants Specifiy Bond Polarity?” in *ACS Symposium Series, Structures and Mechanisms: From Ashes to Enzymes, Proceedings of the Symposium Honoring Professor William Lispcomb on His 80th Birthday* (G.R. Eaton, D.C. Wiley, O. Jardetzky, editors) American Chemical Society, 150-164 (2002)

29. R. J. Bartlett, “Electron Correlation from Molecules to Materials,” in *Electron Correlations and Materials Properties 2* (T. Gonis, N. Kioussis and M. Ciftan, editors), Kluwer Academic, Plenum Publishers, 219-236 (2003).

30. S.A. Fau, R.J. Bartlett, “Changing the Properties of N_5^+ and N_5^- by Substitution” in *Energetic Materials. Part I. Decomposition, Crystal and Molecular Properties* (P. Politzer and J. S. Murray, editors) Elsevier, 441-455 (2003).

31. M. Musial, S.A. Kucharski and R.J. Bartlett, “Approximate inclusion of the T_3 and R_3 operators in the equation-of-motion coupled cluster method,” in *Advances in Quantum Chemistry*, Volume 47, Academic Press, 209-221 (2004).

32. R.J. Bartlett, “On the Evaluation of analytic Energy Derivatives for Correlated Wavefunctions” in *Molecular Quantum Mechanics: Selected Papers of N.C. Handy,* D.C. Clary, S.M. Colwell and H.F. Schaefer III, editors) Taylor & Francis, 127-130 (2004).

33. R.J. Bartlett, D.E. Taylor and A. Korkin, “Achieving Predictive Simulations with Quantum Mechanical Forces via the Transfer Hamiltonian: Problems and Prospects,” in *Handbook of Materials Modeling, Vol. 1: Methods and Models*, Springer, 27-57 (2005).

34. S.A. Perera and R.J. Bartlett, “A Reinvestigation of Ramsey’s Theory of NMR Coupling,” in *Advances in Quantum Chemistry*, Academic Press, 435-467 (2005).

35. R. J. Bartlett, “How and Why Coupled-cluster Theory Became the Pre-eminent Method in *Ab Initio* Quantum Chemistry?” in *Theory and Applications of Computational Chemistry: The First Forty Years,* (C. Dykstra, G. Frenking, K. Kim and G. Scuseria, editors) Elsevier, 1191-1221 (2005).

36. T.M. Henderson, J.C. Greer, G. Bersucker, A. Korkin, and R.J. Bartlett, “Effect of Chemical Environment and Strain on Oxygen Vacancy Formation Energies at Silicon-Silicon Oxide Interfaces,” in *Defects in High-k Gate Dielectric Stacks*, (E. Gustev, editor) Springer, 373-383 (2006).

37. R.J. Bartlett, M. Musial, V. Lotrich, and T. Kuś, “The Yearn to be Hermitian,” in *Recent Progress in Coupled Cluster Methods*, (P. Čársky, J. Paldus, and J. Pittner, editors) Springer, 1-34 (2010).

38. E. Deumens, V.F. Lotrich, A.S. Perera, R.J. Bartlett, N. Jindal, B.A. Sanders, “The super instruction architecture: A framework for high-productivity parallel implementation of coupled-cluster methods on petascale computers,” in *Annual Reports in Computational Chemistry*, Vol. 7, p 179-192, ISBN 978-0-444-53835-2, (Ralph Wheeler, editor) Elsevier, Amsterdam (2011).

39. A. Perera and R.J. Bartlett, “Geometric Metastability in Molecules as a Way to Enhance Energy Storage,” in *Advances in Quantum Chemistry*, volume 69, 147-170, Academic Press (2014).

III. BOOKS – AUTHOR

INDEX TOP

1. I. Shavitt and R.J. Bartlett, *Many-Body Methods in Chemistry and Physics: MBPT and Coupled-Cluster Theory,* Cambridge Press, 2009.

IV. JOURNAL PUBLICATIONS (1ST OF EACH YEAR IN BLUE)

(1970’s)

INDEX TOP

1. R. J. Bartlett and Y. Öhrn, “How quantitative is the concept of maximum overlap?” Theoret. Chim. Acta **21**, 215-234 (1971).
2. R. J. Bartlett and E. J. Brändas, “Geometric sumrule and the reduced partitioning procedure,” Int. J. Quantum Chem. Symp. **5**, 151-159 (1971).
3. E. J. Brändas and R. J. Bartlett, “Reduced partitioning technique for configuration interaction calculations using Padé approximants and inner-projections,” Chem. Phys. Lett. **8**, 153-156 (1971).
4. R. J. Bartlett and E. J. Brändas, “Reduced partitioning procedure in configuration interaction studies. I. Ground states,” J. Chem. Phys. **56**, 5467-5477 (1972).
5. R. J. Bartlett and E. J. Brändas, “Reduced partitioning procedure in configuration interaction studies. II. Excited states,” J. Chem. Phys. **59**, 2032-2042 (1973).

6. R. J. Bartlett, J. C. Bellum and E. J. Brändas, “The treatment of correlation effects in second-order properties,” Int. J. Quantum Chem. Symp. **7**, 449-462 (1973).
7. R. J. Bartlett and D. M. Silver, “Correlation energy in LiH, BH, and HF with many-body perturbation theory using Slater-type atomic orbitals,” Int. J. Quantum Chem. Symp.**8**, 271-276 (1974).
8. R. J. Bartlett and D. M. Silver, “Pair-correlation energies in sodium hydride with many-body perturbation theory,” Phys. Rev. A **10**, 1927-1931 (1974). *Erratum*: Phys. Rev. A **13** (2), 912 (1976).
9. R. J. Bartlett and D. M. Silver, “Many-body perturbation theory applied to hydrogen fluoride,” Chem. Phys. Lett. **29**, 199-203 (1974).
10. R. J. Bartlett and H. Weinstein, “Theoretical treatment of multiple site reactivity in large molecules,” Chem. Phys. Lett. **30**, 441-447 (1975).
11. R. J. Bartlett and D. M. Silver, “Many-body perturbation theory applied to electron pair correlation energies. I. Closed-shell first-row diatomic hydrides,” J. Chem. Phys. **62**, 3258-3268 (1975). *Erratum*: J. Chem. Phys. **64** (3) 1260 (1976).
12. R. J. Bartlett and D. M. Silver, “Some aspects of diagrammatic perturbation theory,” Int. J. Quantum Chem. Symp. **9**, 183-198 (1975).
13. D. M. Silver and R. J. Bartlett, “Modified potentials in many-body perturbation theory,” Phys. Rev. A 13, 1-12 (1976).
14. T.-S. Nee, R. G. Parr and R. J. Bartlett, “Direct determination of the rotational barrier in ethane using perturbation theory,” J. Chem. Phys. **64**, 2216-2225 (1976).
15. G. Blyholder, D. Shihabi, W. V. Wyatt and R. J. Bartlett, “Adsorption and interaction of C_2H_4, H_2,CO and organic acids on Fe, Co, and Ni,” J. Catalysis **43**, 122-130 (1976).
16. R. J. Bartlett and D. M. Silver, “Many-body perturbation theory applied to electron pair correlation energies. II. Closed-shell second row-diatomic hydrides,” J. Chem. Phys. **64**, 4578-4586 (1976).
17. D. D. Koelling, D. E. Ellis and R. J. Bartlett, “Relativistic energy levels and bonding in actinide hexafluorides,” J. Chem. Phys. **65**, 3331-3340 (1976).
18. D. M. Silver, S. Wilson and R. J. Bartlett, “Modified potentials in many-body perturbation theory: three-body and four-body contributions,” Phys. Rev. A **16**, 477-483 (1977).
19. R. J. Bartlett and I. Shavitt, “Comparison of high-order many-body perturbation theory and configuration interaction for H_2O,” Chem. Phys. Lett. **50**, 190-198 (1977).
20. R. J. Bartlett and R. G. Parr, “Polyatomic force constants from charge densities and field gradients,” J. Chem. Phys. **67**, 5828-5837 (1977).
21. R. J. Bartlett and I. Shavitt, “Determination of the size-consistency error in the single and double excitation configuration interaction model,” Int. J. Quantum Chem. Symp. **11**, 165-173 (1977).

22. S. Wilson, D. M. Silver and R. J. Bartlett, “Many-body effects in the $X^1\Sigma^+$ states of the hydrogen fluoride, lithium fluoride and boron fluoride molecules,” Mol. Phys. **33**, 1177-1193 (1977).

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