

## LIST OF PUBLICATIONS<sup>†</sup>

### 1. Monographs, Book Chapters, and Feature Articles<sup>††</sup>

1. P. Piecuch, “Cartesian-Spherical Transformation Formalism and the Theoretical Insight into Many-Body Long-Range Forces of the Electrostatic Origin in Multimolecular Systems,” in: *Interactions of Water in Ionic and Nonionic Hydrates*, edited by H. Kleeberg (Springer, Berlin, 1987), pp. 299-302 [invited book chapter].
2. P. Piecuch, “Towards Classification and Analytical Description of Molecular Interactions Including Quantum-Mechanical Many-Body Effects,” in: *Molecules in Physics, Chemistry and Biology, Topics in Molecular Organization and Engineering*, Vol. 2, *Physical Aspects of Molecular Systems*, edited by J. Maruani (Kluwer, Dordrecht, 1988), pp. 417-505 [monograph, invited book chapter].
3. J. Paldus, P. Piecuch, B. Jeziorski, and L. Pylypow, “Extension of Coupled Cluster Methodology to Open Shells: State Universal Approach,” in: *Recent Progress in Many-Body Theories*, Vol. 3, edited by T. L. Ainsworthy, C. E. Campbell, B. E. Clements, and E. Krotschek (Plenum Press, New York, 1992), pp. 287-303 [invited book chapter].
4. P. Piecuch and R.J. Bartlett, “EOMXCC: A New Coupled-Cluster Method for Electronically Excited States,” *Adv. Quantum Chem.* **34**, 295-380 (1999) [invited book chapter].
- 5.\* P. Piecuch and K. Kowalski, “In Search of the Relationship between Multiple Solutions Characterizing Coupled-Cluster Theories,” in: *Computational Chemistry: Reviews of Current Trends*, edited by J. Leszczynski (World Scientific, Singapore, 2000), Vol. 5, pp. 1-104 [monograph, invited book chapter].
- 6.\* P. Piecuch, K. Kowalski, I.S.O. Pimienta, and S.A. Kucharski, “Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing “Black-Box” Approaches for Molecular Potential Energy Surfaces,” in: *Low-Lying Potential Energy Surfaces*, ACS Symposium Series, Vol. 828, edited by M.R. Hoffmann and K.G. Dyllal (American Chemical Society, Washington, D.C., 2002), pp. 31-64 [invited book chapter].
- 7.\*\* P. Piecuch, K. Kowalski, I.S.O. Pimienta, and M.J. McGuire, “Recent Advances in Electronic Structure Theory: Method of Moments of Coupled-Cluster Equations and Renormalized Coupled-Cluster Approaches,” *Int. Rev. Phys. Chem.* **21**, 527-655 (2002) [invited advanced review].

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<sup>†</sup> Papers written at Michigan State University before submitting the tenure promotion package in the Fall of 2001 are marked by \*. Papers written at Michigan State University after submitting the tenure promotion package in the Fall of 2001 are marked by \*\*

<sup>††</sup> All other invited papers are listed with the remaining original articles.

- 8.\*\* P. Piecuch, I.S.O. Pimienta, P.-F. Fan, and K. Kowalski, "New Alternatives for Electronic Structure Calculations: Renormalized, Extended, and Generalized Coupled-Cluster Theories," in: *Progress in Theoretical Chemistry and Physics*, Vol. 12, *Advanced Topics in Theoretical Chemical Physics*, edited by J. Maruani, R. Lefebvre, and E. Brändas (Kluwer, Dordrecht, 2003), pp. 119-206 [invited advanced review book chapter].
- 9.\*\* P. Piecuch, K. Kowalski, I.S.O. Pimienta, P.-D. Fan, M. Lodriguito, M.J. McGuire, S.A. Kucharski, T. Kuś, and M. Musiał, "Method of Moments of Coupled-Cluster Equations: A New Formalism for Designing Accurate Electronic Structure Methods for Ground and Excited States," *Theor. Chem. Acc.* **112**, 349-393 (2004) [invited overview Feature Article].
- 10.\*\* P. Piecuch, M. Włoch, J.R. Gour, D.J. Dean, M. Hjorth-Jensen, and T. Papenbrock, "Bridging Quantum Chemistry and Nuclear Structure Theory: Coupled-Cluster Calculations for Closed- and Open-Shell Nuclei," in: *Nuclei and Mesoscopic Physics: Workshop on Nuclei and Mesoscopic Physics WNMP 2004*, AIP Conference Proceedings, Vol. 777, edited by V. Zelevinsky (American Institute of Physics, Melville, NY, 2005), pp. 28-45 [invited book chapter in conference proceedings].
- 11.\*\* D.J. Dean, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, M. Włoch, and P. Piecuch, "Coupled Cluster Approaches to Nuclei, Ground States and Excited States," in: *Key Topics in Nuclear Structure, Proceedings of the 8th International Spring Seminar on Nuclear Physics*, edited by A. Covello (World Scientific, Singapore, 2005), pp. 147-157.
- 12.\*\* D.J. Dean, M. Hjorth-Jensen, K. Kowalski, P. Piecuch, and M. Włoch, "Coupled-Cluster Theory for Nuclei," in: *Condensed Matter Theories*, Vol. 20, edited by J.W. Clark, R.M. Panoff, and H. Li (Nova Science Publishers, 2006), pp. XX-XXX [invited book chapter].
- 13.\*\* P. Piecuch, M. Włoch, M. Lodriguito, and J.R. Gour, "Noniterative Coupled-Cluster Methods for Excited Electronic States," in: *Progress in Theoretical Chemistry and Physics*, Vol. 15, "Recent Advances in the Theory of Chemical and Physical Systems," edited by J.-P. Julien, J. Maruani, D. Mayou, S. Wilson, and G. Delgado-Barrio (Springer, Berlin, 2006), pp. 45-106 [invited advanced review book chapter].
- 14.\*\* P.-D. Fan and P. Piecuch, "The Usefulness of Exponential Wave Function Expansions Employing One- and Two-Body Cluster Operators in Electronic Structure Theory: The Extended and Generalized Coupled-Cluster Methods," *Adv. Quantum Chem.* **51**, 1-57 (2006) [invited book chapter].
- 15.\*\* P. Piecuch, M. Włoch, and A.J.C. Varandas, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Application to Potential Function of Water," in: *Progress in Theoretical Chemistry and Physics*, Vol. 16, "Topics in the Theory of Chemical and Physical Systems," edited by S. Lahmar, J. Maruani, S. Wilson, and G. Delgado-Barrio (Springer, Berlin, 2007), pp. 63-121 [invited book chapter].
- 16.\*\* P. Piecuch, I.S.O. Pimienta, P.-D. Fan, and K. Kowalski, "New Alternatives for Accurate Electronic Structure Calculations of Potential Energy Surfaces Involving Bond Breaking," in: *Electron Correlation Methodology*, ACS Symposium Series,

- Vol. 958, edited by A.K. Wilson and K.A. Peterson (American Chemical Society, Washington, D.C., 2007), pp. 37–73 [invited book chapter].
- 17.\*\* J.J. Lutz and P. Piecuch, “Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene,” in: *Nuclei and Mesoscopic Physics, Workshop on Nuclei and Mesoscopic Physics, WNMP 2007*, AIP Conference Proceedings, Vol. 995, edited by P. Danielewicz, P. Piecuch, and V. Zelevinsky (American Institute of Physics, Melville, NY, 2008), pp. 62-71 [invited book chapter in conference proceedings].
  - 18.\*\* M.D. Lodriguito and P. Piecuch, “Method of Moments of Coupled Cluster Equations Employing Multi-Reference Perturbation Theory Wavefunctions: General Formalism, Diagrammatic Formulation, Implementation, and Benchmark Studies,” in: *Progress in Theoretical Chemistry and Physics*, Vol. 18, “Frontiers in Quantum Systems in Chemistry and Physics,” edited by S. Wilson, P. Grout, J. Maruani, G. Delgado-Barrio, and P. Piecuch (Springer, Berlin, 2008), pp. 67-174 [invited book chapter].
  - 19.\*\* W. Li, P. Piecuch, and J.R. Gour, “Local Correlation Calculations Using Standard and Renormalized Coupled-Cluster Methods,” in: *Theory and Applications of Computational Chemistry - 2008*, AIP Conference Proceedings, Vol. 1102, edited by D.-Q. Wei and X.-J. Wang (American Physical Society, Melville, NY, 2009), pp. 68-113 [invited book chapter in conference proceedings].
  - 20.\*\* W. Li, P. Piecuch, and J.R. Gour, “Linear Scaling Local Correlation Extensions of the Standard and Renormalized Coupled-Cluster Methods,” in: *Progress in Theoretical Chemistry and Physics*, Vol. 19, “Advances in the Theory of Atomic and Molecular Systems: Conceptual and Computational Advances in Quantum Chemistry,” edited by P. Piecuch, J. Maruani, G. Delgado-Barrio, and S. Wilson (Springer, Berlin, 2009), pp. 131-195, in press [invited book chapter].

## 2. Articles

21. P. Piecuch, “Invariance Properties of the Multipole Expansion,” *Int. J. Quantum Chem.* **22**, 293-298 (1982).
22. P. Piecuch, “Spherical Tensor Theory of Long-Range Interactions between Two Molecules,” *Int. J. Quantum Chem.* **25**, 449-473 (1984).
23. P. Piecuch, “Higher-Order Contributions to the Intermolecular Energy in the Perturbation Treatment of Long-Range Forces in the Light of Spherical Tensor Theory,” *Chem. Phys. Lett.* **106**, 364-372 (1984).
24. P. Piecuch, “Spherical Multipole Moments and Polarizabilities of Tetrahedral and Octahedral Molecules,” *Acta Phys. Pol. A* **66**, 69-80 (1984).
25. P. Piecuch, “The Non-Additivity of Long-Range Interactions in Second-Order Perturbation Theory in the Light of Spherical Tensor Formalism,” *Chem. Phys. Lett.* **110**, 496-503 (1984).

26. M.M. Szcześniak, Z. Latajka, P. Piecuch, H. Ratajczak, W.J. Orville-Thomas, and C.N.R. Rao, "Theoretical Studies of Lithium Bonding in Lithium Chloride/Aliphatic Amine Complexes," *Chem. Phys.* **94**, 55-63 (1985).
27. P. Piecuch, "Note on the Multipole Expansion in the Spherical Tensor Form," *J. Phys. A: Math. Gen.* **18**, L739-L743 (1985).
28. P. Piecuch, "Supplement to Spherical Tensor Theory of Long-Range Interactions between Two Molecules," *Int. J. Quantum Chem.* **28**, 375-386 (1985).
29. P. Piecuch, "Higher-Order Interaction Energies for a System of  $N$  Arbitrary Molecules in the Light of Spherical Tensor Theory," *J. Math. Phys.* **27**, 2165-2187 (1986).
30. P. Piecuch, "Spherical Tensor Theory of Long-Range Interactions in a System of  $N$  Arbitrary Molecules Including Quantum-Mechanical Many-Body Effects. I. Anisotropic Induction Interactions in the First Three Orders of Perturbation Theory," *Mol. Phys.* **59**, 1067-1083 (1986).
31. P. Piecuch, "Spherical Tensor Theory of Long-Range Interactions in a System of  $N$  Arbitrary Molecules Including Quantum-Mechanical Many-Body Effects. II. Anisotropic Dispersion Interactions in the First Three Orders of Perturbation Theory," *Mol. Phys.* **59**, 1085-1095 (1986).
32. P. Piecuch, "Spherical Tensor Theory of Long-Range Interactions in a System of  $N$  Arbitrary Molecules Including Quantum-Mechanical Many-Body Effects. III. Isotropic Interactions in the First Three Orders of Perturbation Theory," *Mol. Phys.* **59**, 1097-1111 (1986).
33. P. Piecuch, "On the Addition Theorems for Solid Spherical Harmonics," *Rep. Math. Phys.* **24**, 187-192 (1986).
34. P. Piecuch, "Classification of Two- and Many-Body Fourth-Order Induction Interaction Energies in an Arbitrary Multimolecular System," *Acta Phys. Pol. A* **74**, 563-572 (1988).
35. P. Piecuch, "Spherical Tensor Theory of Long-Range Interactions in a System of  $N$  Arbitrary Molecules Including Quantum-Mechanical Many-Body Effects. IV. The Use of Cartesian-Spherical Transformation Formalism," *Mol. Phys.* **66**, 805-818 (1989).
36. P. Piecuch and J. Paldus, "Orthogonally Spin-Adapted Coupled-Cluster Equations Involving Singly and Doubly Excited Clusters. Comparison of Different Procedures for Spin-Adaptation," *Int. J. Quantum Chem.* **36**, 429-453 (1989).
37. P. Piecuch, "Spherical Tensor Theory of Long-Range Interactions in a System of  $N$  Arbitrary Molecules Including Quantum-Mechanical Many-Body Effects. V. Fourth-Order Induction Forces and Scalar Angular Functions for Many-Body Interactions," *Acta Phys. Pol. A* **77**, 453-484 (1990).
38. P. Piecuch and J. Paldus, "Coupled Cluster Approaches with an Approximate Account of Triexcitations and the Optimized Inner Projection Technique. I. General Orthogonally Spin-Adapted Formalism," *Theor. Chim. Acta* **78**, 65-128 (1990).
39. P. Piecuch, S. Zarrabian, J. Paldus, and J. Čížek, "Coupled Cluster Approaches with an Approximate Account of Triexcitations and the Optimized Inner Projection

- Technique. II. Coupled Cluster Results for Cyclic Polyene Model Systems,” *Phys. Rev. B* **42**, 3351-3379 (1990).
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  42. P. Piecuch and J. Paldus, “On the Solution of Coupled-Cluster Equations in the Fully Correlated Limit of Cyclic Polyene Model,” *Int. J. Quantum Chem.: Quantum Chem. Symp.* **25**, 9-34 (1991).
  43. J. Paldus and P. Piecuch, “Electron Correlation in One Dimension: Coupled Cluster Approaches to Cyclic Polyene  $\pi$ -Electron Models,” *Int. J. Quantum Chem.* **42**, 135-164 (1992) [invited paper in a special issue devoted to “Hartree-Fock-Based Correlation Treatments of Extended Systems”].
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  47. P. Piecuch, “MAPLE Symbolic Computation of the Long-Range Many-Body Intermolecular Potentials. Three-Body Induction Forces between Two Atoms and a Linear Molecule,” *Int. J. Quantum Chem.* **47**, 261-305 (1993).
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  50. M.M. Szcześniak, G. Chałasiński, and P. Piecuch, “The Non-Additive Interactions in the  $Ar_2HF$  and  $Ar_2HCl$  Clusters: An *Ab Initio* Study,” *J. Chem. Phys.* **99**, 6732-6741 (1993).
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55. X. Li, P. Piecuch, and J. Paldus, "A Study of <sup>1</sup>A<sub>1</sub> – <sup>3</sup>B<sub>1</sub> Separation in CH<sub>2</sub> Using Orthogonally Spin-Adapted State-Universal and State-Specific Coupled-Cluster Methods," *Chem. Phys. Lett.* **224**, 267-274 (1994).
56. P. Piecuch and J. Paldus, "Orthogonally Spin-Adapted State-Universal Coupled-Cluster Formalism: Implementation of the Complete Two-Reference Theory Including Cubic and Quartic Coupling Terms," *J. Chem. Phys.* **101**, 5875-5890 (1994).
57. P. Piecuch, X. Li, and J. Paldus, "An *Ab Initio* Determination of <sup>1</sup>A<sub>1</sub> – <sup>3</sup>B<sub>1</sub> Energy Gap in CH<sub>2</sub> Using Orthogonally Spin-Adapted State-Universal and State-Specific Coupled-Cluster Methods," *Chem. Phys. Lett.* **230**, 377-386 (1994).
58. P. Piecuch and L. Adamowicz, "Breaking Bonds with the State-Selective Multi-Reference Coupled-Cluster Method," *J. Chem. Phys.* **102**, 898-904 (1995).
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63. K.B. Ghose, P. Piecuch, and L. Adamowicz, "Improved Computational Strategy for the State-Selective Coupled-Cluster Theory with Semiinternal Triexcited Clusters: Potential Energy Surface of HF Molecule," *J. Chem. Phys.* **103**, 9331-9346 (1995).
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65. V. Špirko, P. Piecuch, A.E. Kondo, and J. Paldus, "Molecular Quadrupole Moment Functions of HF and N<sub>2</sub>. II. Rovibrational Effects," *J. Chem. Phys.* **104**, 4716-4727 (1996).

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70. P. Piecuch and J. Paldus, "The Convergence of Energy Expansions for Molecules in Electrostatic Fields: A Linear Response Coupled-Cluster Study," *J. Math. Chem.* **21**, 51-70 (1997).
71. P. Piecuch, "Potential Energy Curves for the  $\text{HF}^-$  and  $\text{CH}_3\text{F}^-$  Anions: A Coupled Cluster Study," *J. Molec. Struct.* **436-437**, 503-536 (1997) [invited contribution in a special issue in honor of Professor Henryk Ratajczak entitled "Structure, Properties, and Dynamics of Molecular Systems," edited by A.J. Barnes and Z. Latajka].
72. X.Y. Chang, R. Ehlich, A.J. Hudson, P. Piecuch, and J.C. Polanyi, "Dynamics of Harpooning Studied by Transition State Spectroscopy. I.  $\text{Na} \cdot \cdot \text{FH}$ ," *Faraday Discuss. Chem. Soc.* **108**, 411-425 (1997) [in response to an invitation issued to J.C. Polanyi].
73. X.Y. Chang, A.J. Hudson, P. Piecuch, and J.C. Polanyi, "Communication on REMPI Two-Photon Ionization Experiment for  $\text{NaF}$ ," included in *General Discussion* (pp. 427-467) of *Faraday Discuss. Chem. Soc.*, *Faraday Discuss. Chem. Soc.* **108**, 463 (1997) [communicated by A.J. Hudson and J.C. Polanyi].
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- 93.\* J.I. Landman and P. Piecuch, "Parallelization of a Legacy Research Program Using OpenMP," *Fortran Forum* **19**, 16-23 (2000).
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## LIST OF EDITED JOURNAL ISSUES AND BOOKS<sup>†</sup>

1. *International Journal of Quantum Chemistry*, Volume 107, Issue 14 (2007). Special Issue: Proceedings from the Eleventh European Workshop on Quantum Systems in Chemistry and Physics (St. Petersburg, Russia, August 20-25, 2006). Issue Edited by Oleg Vasyutinskii, Jean Maruani, Piotr Piecuch, Gerardo Delgado-Barrio, and Stephen Wilson. Preface: *Int. J. Quantum Chem.* **107** (14), 2565-2566 (2007). List of Participants: *Int. J. Quantum Chem.* **107** (14), 2567-2574 (2007).
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5. *Progress in Theoretical Chemistry and Physics* (book series published by Springer), Volume 20 (2009), "Advances in the Theory of Atomic and Molecular Systems: Dynamics, Spectroscopy, Clusters, and Nanostructures." Proceedings from the Thirteenth International Workshop on Quantum Systems in Chemistry and Physics (Lansing, Michigan, U.S.A., July 6-12, 2008). Edited by P. Piecuch, J. Maruani, G. Delgado-Barrio, and S. Wilson.

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<sup>†</sup> Excluding memberships of editorial boards, which are listed in section Editorial Boards of Curriculum Vitae.

## LIST OF INVITED TALKS AT NATIONAL AND INTERNATIONAL SYMPOSIA<sup>†</sup>

1. "Application of the Hilbert-Space Coupled-Cluster Theory to Electronic States of the H<sub>4</sub> Model System," Workshop "Coupled Clusters in the Theory of Atoms and Molecules," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Poland, October 23-24, 1992.
2. "Linear Response Coupled-Cluster Approach to Static Molecular Properties," The symposium "Frontiers in Electronic Structure Theory," 213th American Chemical Society National Meeting, San Francisco, California, U.S.A., April 13-17, 1997.
3. "Coupled-Cluster Approach to Static Molecular Properties," "Coupled Cluster Theory and Electron Correlation" workshop, "Fifty Years of the Correlation Problem," Cedar Key, Florida, U.S.A., June 15-19, 1997, a satellite meeting of the 9th International Congress of Quantum Chemistry, Atlanta, Georgia, U.S.A., June 9-14, 1997.
- 4.\* "Single-Reference Coupled-Cluster Methods for Quasi-Degenerate Electronic States," The symposium "Electronic Structure Theory: From Methods to Molecules and Materials," 100th Annual Meeting of the American Physical Society, Atlanta, Georgia, U.S.A., March 21-26, 1999.
- 5.\* "Dynamics of Harpooning in van der Waals Molecules," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999.
- 6.\* "Dynamics of Harpooning in van der Waals Molecules," "Vth International Conference on Molecular Spectroscopy," Łądek-Zdrój, Poland, September 26-30, 1999.
- 7.\* "Method of Moments of Coupled-Cluster Equations: A New Approach to the Many-Electron Correlation Problem," The 2000 Florida Award Symposium (honoring Dr. Rodney J. Bartlett's work), FAME 2000 (Florida Annual Meeting and Exposition, organized by the Florida Section of the American Chemical Society), Orlando, Florida, U.S.A., May 12, 2000.
- 8.\* "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Joint Polish-German Conference on Modern Optics: Fundamental Aspects of Spectroscopy and Environmental Applications, Jurata near Gdańsk, Poland, September 17-22, 2000.
- 9.\* "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," the 41st Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 24-March 2, 2001.

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<sup>†</sup> Invited talks at symposia that Dr. P. Piecuch gave after joining Michigan State University in August 1998 and before submitting the tenure promotion package in the Fall of 2001 are marked by \*. Invited talks at symposia that Dr. P. Piecuch gave after submitting the tenure promotion package in the Fall of 2001 are marked by \*\*. Invited talks given by co-authors at conferences are listed with papers presented at conferences.

- 10.\* “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces,” First Southern School on Computational Chemistry (one of the two formal lectures), Orange Beach, Alabama, March 23-24, 2001.
- 11.\* “Effect of the Potential Energy Surface on the Dynamics of Weakly Bound Precursor Complexes and New “Black-Blox” Coupled-Cluster Methods for Entire Potential Energy Surfaces of Reactive Molecular Systems,” The symposium “First Principles Chemical Reaction Dynamics,” 222nd American Chemical Society National Meeting, Chicago, Illinois, U.S.A., August 26–30, 2001.
- 12.\* “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” 34th Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, Minnesota, U.S.A., October 5–6, 2001.
- 13.\*\* “Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Quasi-Degenerate Ground States, Molecular Potential Energy Surfaces, and Excited States,” Institute for Nuclear Theory workshop on “Advanced Computational Methods for Solving the Nuclear Many-Body Problem,” Seattle, Washington, U.S.A., March 12–15, 2002.
- 14.\*\* “New Single- and Multi-Reference Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” The symposium “Recent Advances in Electron Correlation Methodology,” 223rd American Chemical Society National Meeting, Orlando, Florida, U.S.A., April 7–11, 2002.
- 15.\*\* “Method of Moments of Coupled-Cluster Equations: A New Framework for Designing Accurate Electronic Structure Methods,” Fourth International Congress of the International Society for Theoretical Chemical Physics (ICTCP-IV), Marly-le-Roi near Paris, France, July 9-16, 2002 [invited plenary lecture].
- 16.\*\* “Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate Electronic Structure Methods,” International Symposium on Frontiers in Molecular Science 2002, Qingdao, China, July 15-18, 2002.
- 17.\*\* “Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” 6th World Congress of Theoretically Oriented Chemists (WATOC02), Lugano, Switzerland, August 4-9, 2002 [invited contributed talk].
- 18.\*\* “Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate (Virtually Exact) and Inexpensive Electronic Structure Methods,” 11th Conference on Current Trends in Computational Chemistry, Jackson, Mississippi, U.S.A., November 1-2, 2002.
- 19.\*\* “New Alternatives for Accurate Electronic Structure Calculations of Molecular Potential Energy Surfaces,” The symposium “New Electronic Structure Methods: From Molecules to Materials,” 225th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., March 23-27, 2003.

- 20.\*\* "Single- and Multi-reference Coupled-Cluster Methods for Quasidegenerate Electronic States and Bond Breaking," The symposium "Bond-Breaking Methods in Gas and Condensed Phases," 226th American Chemical Society National Meeting, New York, New York, U.S.A., September 7-11, 2003.
- 21.\*\* "Noniterative Coupled-Cluster Methods for Accurate Calculations of Excited Electronic States," The symposium "The Systematic Treatment of Electron Correlation. A Celebration of the Science of Rodney J. Bartlett," St. Simons Island, Georgia, U.S.A., April 23-25, 2004.
- 22.\*\* "Coupled-Cluster Method: An Accurate Ab Initio Theory of Atoms, Molecules, Nuclei, and Other Many-Fermion Systems," International Workshop on Microscopic Approaches to Nuclear Structure Calculations," UMIST, Manchester, U.K., July 4-8, 2004.
- 23.\*\* "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Workshop "New Perspectives on p-Shell Nuclei," Michigan State University, East Lansing, U.S.A., July 22-24, 2004.
- 24.\*\* "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," International conference "Molecular Quantum Mechanics: the No Nonsense Path to Progress" honoring Professor Nicholas Handy's work, St. John's College, Cambridge University, Cambridge, U.K., July 24-29, 2004.
- 25.\*\* "Renormalized Coupled-Cluster Methods and their Automated Parallel Computer Implementation with Tensor Contraction Engine," The symposium "Symbolic Calculation in Chemistry," 228th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 22-26, 2004.
- 26.\*\* "Coupled Cluster Calculations of Ground and Excited States of Nuclei," International Conference on Exotic Nuclei and Atomic Masses, ENAM-04, Pine Mountain, Georgia, September 12-16, 2004.
- 27.\*\* "Non-Iterative Coupled-Cluster Methods For Accurate Calculations of Excited Electronic States," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004.
- 28.\*\* "Coupled Cluster Calculations of Ground and Excited States of Nuclei," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004.
- 29.\*\* "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Institute for Nuclear Theory workshop "Microscopic Nuclear Structure Theory," "Nuclear Forces and the Quantum Many-Body Problem," Seattle, Washington, U.S.A., October 4-8, 2004.
- 30.\*\* "Coupled-Cluster Method: Highly Accurate Microscopic Approach to Molecular Systems and Nuclei," Workshop "Nuclei and Mesoscopic Physics," Michigan State University, East Lansing, U.S.A., October 23-26, 2004.
- 31.\*\* "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," 7th World Congress of Theoretically Oriented Chemists (WATOC05), Cape Town, South Africa, January 16-21, 2005.

- 32.\*\* “Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Electronic Quasi-Degeneracies and Open-Shell Problems,” Fifth Congress of the International Society for Theoretical Chemical Physics (ICTCP-V), New Orleans, Louisiana, U.S.A., July 20-26, 2005.
- 33.\*\* “Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States,” The symposium “Theoretical Determination of Energy Landscapes: Methodology and Applications,” 230th American Chemical Society National Meeting, Washington, DC, U.S.A., August 28-September 1, 2005.
- 34.\*\* “Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Quasi-Degeneracies and Open-Shell Problems,” Conference on Microscopic Approaches to Many-Body Theory, in honor of Professor Raymond Bishop, The University of Manchester, Manchester, U.K., August 31-September 3, 2005.
- 35.\*\* “Active-Space Coupled-Cluster Method: An Inexpensive and Highly Accurate Approach to Electronic Quasi-Degeneracies and Open-Shell Problems,” Tenth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-X, Carthage, Tunisia, September 1-7, 2005.
- 36.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006.
- 37.\*\* “Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Electronic Excitations in Molecules to Properties of Atomic Nuclei,” The Centro Internacional de Matemática Workshop “Mathematics in Chemistry,” Lisbon, Portugal, July 19-21, 2006.
- 38.\*\* “Advances in Electronic Structure Theory: Single-Reference Coupled-Cluster Methods for Multi-Reference Problems,” Sixth Canadian Computational Chemistry Conference (CCCC6), Vancouver, Canada, July 26-30, 2006 [invited plenary lecture].
- 39.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” Eleventh European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XI, St. Petersburg, Russia, August 20-25, 2006.
- 40.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” International Conference “Recent Trends in Many-Body Methods for Electronic Structure and Properties of Atoms and Molecules,” Bhubaneswar and Puri, Orissa, India, January 11-13, 2007.
- 41.\*\* “Active-Space Coupled-Cluster Methods for Bond Breaking, Excited Electronic States, and Open-Shell Systems,” International Conference “Practicing Chemistry with Theoretical Tools, on the Occasion of Professor Mark S. Gordon’s 65th Birthday,” Kihei, Hawaii, U.S.A., January 15-18, 2007.
- 42.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007.

- 43.\*\* "Coupled-Cluster Theory: An Overview of the Basic Formalism and Applications to Molecular and Nuclear Structure Problems," Workshop on Advanced Many-body Methods for Nuclear Structure European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 2-6, 2007.
- 44.\*\* "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, and Bond Breaking," Twelfth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XII, London, U.K., August 30 - September 5, 2007.
- 45.\*\* "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, Reaction Pathways, and Photochemistry," "IXth International Conference on Molecular Spectroscopy: From Molecules to Molecular Biological Systems and Molecular Materials: Role of Molecular Interactions and Recognition," Wrocław – Łądek-Zdrój, Poland, September 12-16, 2007.
- 46.\*\* "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell Systems," The symposium "Electronic Structure and Reaction Dynamics of Open-shell Species," 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., April 6-10, 2008.
- 47.\*\* "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," Sixth Congress of the International Society for Theoretical Chemical Physics (ICTCP-VI), Vancouver, British Columbia, Canada, July 19-24, 2008 [invited plenary lecture].
- 48.\*\* "Coupled-Cluster Theory: A Brief Overview of Modern Methods and Applications to Nuclear Structure," the WE-Heraeus-Seminar "Ab-Initio Nuclear Structure - Where do we stand?", Bad Honnef, Germany, July 28-30, 2008.
- 49.\*\* "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008.
- 50.\*\* "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," The International Conference on the Theory and Applications of Computational Chemistry in 2008 (TACC 2008), Shanghai, China, September 23-27, 2008 [invited plenary lecture].
- 51.\*\* "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," The symposium "Advances in Electronic Structure Theory and First Principles Dynamics," 237th American Chemical Society National Meeting, Salt Lake City, Utah, U.S.A., March 22-26, 2009.
- 52.\*\* "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States," 30th Annual Combustion Research Meeting, Airlie Conference Center, Warrenton, Virginia, May 26-29, 2009.

- 53.\*\* “Coupled-Cluster Theory: From Quantum Chemistry to Applications in Nuclear Physics,” International Workshop “Linking Nuclei, Molecules, and Condensed Matter: Computational Quantum Many-Body Approaches,” European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 6-10, 2009.
- 54.\*\* “Dealing with Strong Electron Correlations in Quantum Chemistry via Renormalized, Active-Space, and Multi-Reference Coupled-Cluster Methods,” The symposium “New Developments in Strongly Correlated Electrons,” 238th American Chemical Society National Meeting, Washington, DC, U.S.A., August 16-20, 2009.
- 55.\*\* “Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies,” Fourteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XIV, San Lorenzo del Escorial, Madrid, Spain, September 13-19, 2009.
- 56.\*\* TBA, International conference on “Recent Advances in Many-Electron Theories,” Raman Center for the Atomic, Molecular, and Optical Sciences, Indian Association for the Cultivation of Science, Kolkata, India, January 4-6, 2010.
- 57.\*\* TBA, 10-minute perspective talk preceding a session on multi-reference coupled-cluster theory, the 50th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 24-March 2, 2010.
- 58.\*\* TBA, International conference “Molecular Quantum Mechanics: From Methylene to DNA and Beyond” honoring Professor Henry F. Schaefer’s work, University of California at Berkeley, Berkeley, California, May 24-29, 2010.

In addition, Dr. Piotr Piecuch has been invited to present a paper “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces” at the 262nd WE-Heraeus-Seminar entitled “Modern Aspects of Many-Electron Theory,” Bad Honnef, Germany, October 21–24, 2001 [classified as invited poster].

## LIST OF ALL INVITED TALKS<sup>†</sup>

1. "Invariance Properties of the Multipole Expansion," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Poland, May 12, 1983.
2. "What Was Most Fascinating for Me in my Master of Science Research Project and will I Continue this Kind of Research in the Future," The Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Katowice, Poland, September 22, 1983 [lecture on the occasion of receiving the Individual Prize of the Polish Chemical Society].
3. "Irreducible Tensor Operators in Theory of Long-Range Intermolecular Interactions," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Poland, April 5, 1984.
4. "Perturbation-Theoretical Description of Long-Range Intermolecular Interactions - the Application of Racah-Wigner Algebra and the Formalism of Irreducible Tensors," Non-linear Optics Division, Institute of Physics, University of Poznań, Poland, March 29, 1988.
5. "Orthogonally Spin-Adapted Multi-Reference Coupled-Cluster Theory and Its Application to Model Systems with Varying Degree of Quasidegeneracy," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Poland, December 5, 1991.
6. "Application of the Hilbert-Space Coupled-Cluster Theory to Electronic States of the H<sub>4</sub> Model System," Workshop "Coupled Clusters in the Theory of Atoms and Molecules," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Poland, October 23-24, 1992.
7. "Recent Progress in Coupled Cluster Theory," Physical Chemistry Division Seminar, Department of Chemistry, University of Arizona, Tucson, Arizona, U.S.A., September 27, 1993.
8. "Recent Progress in Coupled Cluster Theory," Department of Chemistry, Indiana University, Bloomington, Indiana, U.S.A., January 3, 1994.
9. "Linear Response Coupled-Cluster Approach to Static Molecular Properties," The symposium "Frontiers in Electronic Structure Theory," 213th American Chemical Society National Meeting, San Francisco, California, U.S.A., April 13-17, 1997 [co-authors: A.E. Kondo, J. Paldus, and V. Špirko].
10. "Electron Correlation in Chemical Bonding," Department of Chemistry, York University, North York, Ontario, Canada, March, 1996.

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<sup>†</sup> Invited talks that Dr. P. Piecuch gave after joining Michigan State University in August 1998 and before submitting the tenure promotion package in the Fall of 2001 are marked by \*. Invited talks that Dr. P. Piecuch gave after submitting the tenure promotion package in the Fall of 2001 are marked by \*\*. Invited talks given by co-authors at conferences are listed with papers presented at conferences.

11. "Coupled-Cluster Approach to Static Molecular Properties," "Coupled Cluster Theory and Electron Correlation" workshop, "Fifty Years of the Correlation Problem," Cedar Key, Florida, U.S.A., June 15-19, 1997, a satellite meeting of the 9th International Congress of Quantum Chemistry, Atlanta, Georgia, U.S.A., June 9-14, 1997.
12. "Electron Correlation in Molecules," Special Physical Chemistry Seminar, Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., August 14, 1997.
13. "Dynamics of Harpooning in van der Waals Molecules," Department of Chemistry, Michigan State University, East Lansing, Michigan, U.S.A., December 16, 1997.
14. "Dynamics of Harpooning in van der Waals Molecules," Quantum Theory Project Seminar, Quantum Theory Project, University of Florida, Gainesville, Florida, U.S.A., March 18, 1998.
- 15.\* "Single-Reference Coupled-Cluster Methods for Quasi-Degenerate Electronic States," The symposium "Electronic Structure Theory: From Methods to Molecules and Materials," 100th Annual Meeting of the American Physical Society, Atlanta, Georgia, U.S.A., March 21-26, 1999.
- 16.\* "Coupled-Cluster Theory: A Powerful Approach to Many-Electron Correlation Problem," Departmental Seminar, Department of Chemistry, University of Minnesota, Minneapolis, Minnesota, U.S.A., April 26, 1999.
- 17.\* "Dynamics of Harpooning in van der Waals Molecules," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999.
- 18.\* "Dynamics of Harpooning in van der Waals Molecules," "Vth International Conference on Molecular Spectroscopy," Łądek-Zdrój, Poland, September 26-30, 1999.
- 19.\* "Method of Moments of Coupled-Cluster Equations: A New Approach to the Many-Electron Correlation Problem," Quantum Theory Seminar, Department of Applied Mathematics, University of Waterloo, Waterloo, Ontario, Canada, May 4, 2000.
- 20.\* "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Chemical Physics Research Seminar, Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada, May 5, 2000.
- 21.\* "Method of Moments of Coupled-Cluster Equations: A New Approach to the Many-Electron Correlation Problem," The 2000 Florida Award Symposium (honoring Dr. Rodney J. Bartlett's work), FAME 2000 (Florida Annual Meeting and Exposition, organized by the Florida Section of the American Chemical Society), Orlando, Florida, U.S.A., May 12, 2000.
- 22.\* "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Joint Polish-German Conference on Modern Optics: Fundamental Aspects of Spectroscopy and Environmental Applications, Jurata near Gdańsk, Poland, September 17-22, 2000.

- 23.\* “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Poland, September 29, 2000.
- 24.\* “Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules,” Department of Chemistry, University of Arizona, Tucson, Arizona, U.S.A., October 23, 2000.
- 25.\* “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces,” the 41st Sani-bel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 24-March 2, 2001.
- 26.\* “Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules,” Department of Chemistry and Computational Center for Molecular Structure and Interactions, Distinguished Lecture Series in Computational Chemistry and Physics, Jackson State University, Jackson, Mississippi, U.S.A., March 23, 2001.
- 27.\* “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces,” First Southern School on Computational Chemistry (one of the two formal lectures), Orange Beach, Alabama, March 23-24, 2001.
- 28.\* “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces,” NSCL Theory Journal Club, National Superconducting Cyclotron Laboratory, Michigan State University, June 22 and 26, 2001.
- 29.\* “Effect of the Potential Energy Surface on the Dynamics of Weakly Bound Precursor Complexes and New “Black-Blox” Coupled-Cluster Methods for Entire Potential Energy Surfaces of Reactive Molecular Systems,” The symposium “First Principles Chemical Reaction Dynamics,” 222nd American Chemical Society National Meeting, Chicago, Illinois, U.S.A., August 26–30, 2001.
- 30.\* “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” 34th Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, Minnesota, U.S.A., October 5–6, 2001.
- 31.\* “Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules,” Institute of Physical and Theoretical Chemistry, Department of Chemistry, Wrocław University of Technology, Wrocław, Poland, October 19, 2001.
- 32.\* “Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” J. Heyrovský Institute of Physical Chemistry, Academy of Sciences of the Czech Republic, Prague, Czech Republic, October 26, 2001.
- 33.\*\* “Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” Department of Chemistry, University of Wrocław, Wrocław, Poland, November 9, 2001.
- 34.\*\* “Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” Condensed Matter Physics Seminar, Department of Physics and Astronomy, Michigan State University, November 29, 2001.

- 35.\*\* “Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” Department of Chemistry, Iowa State University, Ames, Iowa, U.S.A., March 6, 2002.
- 36.\*\* “Advances in Electronic Structure Theory: Multi-Reference Coupled-Cluster Methods,” Scalable Computing Laboratory, Ames Laboratory, USDOE, Iowa State University, Ames, Iowa, U.S.A., March 7, 2002.
- 37.\*\* “Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Quasi-Degenerate Ground States, Molecular Potential Energy Surfaces, and Excited States,” Institute for Nuclear Theory workshop on “Advanced Computational Methods for Solving the Nuclear Many-Body Problem,” Seattle, Washington, U.S.A., March 12–15, 2002.
- 38.\*\* “New Single- and Multi-Reference Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” The symposium “Recent Advances in Electron Correlation Methodology,” 223rd American Chemical Society National Meeting, Orlando, Florida, U.S.A., April 7–11, 2002.
- 39.\*\* “Method of Moments of Coupled-Cluster Equations: A New Framework for Designing Accurate Electronic Structure Methods,” Fourth International Congress of the International Society for Theoretical Chemical Physics (ICTCP-IV), Marly-le-Roi near Paris, France, July 9-16, 2002 [invited plenary lecture].
- 40.\*\* “Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate Electronic Structure Methods,” International Symposium on Frontiers in Molecular Science 2002, Qingdao, China, July 15-18, 2002.
- 41.\*\* “Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States,” 6th World Congress of Theoretically Oriented Chemists (WATOC02), Lugano, Switzerland, August 4-9, 2002 [invited contributed talk].
- 42.\*\* “Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate (Virtually Exact) and Inexpensive Electronic Structure Methods,” 11th Conference on Current Trends in Computational Chemistry, Jackson, Mississippi, U.S.A., November 1-2, 2002.
- 43.\*\* “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited Electronic States,” Lawrence Livermore National Laboratory, Livermore, California, U.S.A., November 13, 2002.
- 44.\*\* “New Ideas in Electronic Structure Theory: Method of Moments of Coupled-Cluster Equations,” Department of Chemistry, University of California at Berkeley, Berkeley, California, U.S.A., November 15, 2002.
- 45.\*\* “New Ideas in Electronic Structure Theory: Method of Moments of Coupled-Cluster Equations,” Department of Chemistry, University of North Dakota, Grand Forks, North Dakota, U.S.A., November 21, 2002.

- 46.\*\* "New Ideas in Electronic Structure Theory: Method of Moments of Coupled-Cluster Equations," Department of Chemistry, North Dakota State University, Fargo, North Dakota, U.S.A., November 22, 2002.
- 47.\*\* "New Alternatives for Accurate Electronic Structure Calculations of Molecular Potential Energy Surfaces," Department of Chemistry, Ohio State University, Columbus, Ohio, U.S.A., December 5, 2002.
- 48.\*\* "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited Electronic States," National Superconducting Cyclotron Laboratory, Michigan State University, March 20, 2003.
- 49.\*\* "New Alternatives for Accurate Electronic Structure Calculations of Molecular Potential Energy Surfaces," The symposium "New Electronic Structure Methods: From Molecules to Materials," 225th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., March 23-27, 2003.
- 50.\*\* "Single- and Multi-reference Coupled-Cluster Methods for Quasidegenerate Electronic States and Bond Breaking," The symposium "Bond-Breaking Methods in Gas and Condensed Phases," 226th American Chemical Society National Meeting, New York, New York, U.S.A., September 7-11, 2003.
- 51.\*\* "New Alternatives for Accurate Electronic Structure Calculations for Molecular Systems," Department of Chemistry and Biochemistry, Southern Illinois University at Carbondale, Carbondale, Illinois, U.S.A., October 3, 2003.
- 52.\*\* "New Alternatives for Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems," Department of Physics, Central Michigan University, Mount Pleasant, Michigan, U.S.A., March 18, 2004.
- 53.\*\* "Noniterative Coupled-Cluster Methods for Accurate Calculations of Excited Electronic States," The symposium "The Systematic Treatment of Electron Correlation. A Celebration of the Science of Rodney J. Bartlett," St. Simons Island, Georgia, U.S.A., April 23-25, 2004.
- 54.\*\* "Coupled-Cluster Method: An Accurate Ab Initio Theory of Atoms, Molecules, Nuclei, and Other Many-Fermion Systems," International Workshop on Microscopic Approaches to Nuclear Structure Calculations," UMIST, Manchester, U.K., July 4-8, 2004.
- 55.\*\* "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Workshop "New Perspectives on p-Shell Nuclei," Michigan State University, East Lansing, U.S.A., July 22-24, 2004.
- 56.\*\* "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," International conference "Molecular Quantum Mechanics: the No Nonsense Path to Progress" honoring Professor Nicholas Handy's work, St. John's College, Cambridge University, Cambridge, U.K., July 24-29, 2004.
- 57.\*\* "Renormalized Coupled-Cluster Methods and their Automated Parallel Computer Implementation with Tensor Contraction Engine," The symposium "Symbolic Calculation in Chemistry," 228th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 22-26, 2004.

- 58.\*\* "Coupled Cluster Calculations of Ground and Excited States of Nuclei," International Conference on Exotic Nuclei and Atomic Masses, ENAM-04, Pine Mountain Georgia, September 12-16, 2004.
- 59.\*\* "Non-Iterative Coupled-Cluster Methods For Accurate Calculations of Excited Electronic States," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004.
- 60.\*\* "Coupled Cluster Calculations of Ground and Excited States of Nuclei," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004.
- 61.\*\* "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Institute for Nuclear Theory workshop "Microscopic Nuclear Structure Theory," "Nuclear Forces and the Quantum Many-Body Problem," Seattle, Washington, U.S.A., October 4-8, 2004.
- 62.\*\* "New Alternatives for Accurate Quantum Calculations for Molecular Systems: Bond Breaking, Diradicals, and Excited Electronic States," Department of Physical Chemistry, University of Geneva, Switzerland, October 15, 2004.
- 63.\*\* "Coupled-Cluster Method: Highly Accurate Microscopic Approach to Molecular Systems and Nuclei," Workshop "Nuclei and Mesoscopic Physics," Michigan State University, East Lansing, U.S.A., October 23-26, 2004.
- 64.\*\* "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," 7th World Congress of Theoretically Oriented Chemists (WATOC05), Cape Town, South Africa, January 16-21, 2005.
- 65.\*\* "New Alternatives for Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Diradicals to Excited Electronic States in Molecules and Atomic Nuclei," Department of Chemistry, Wayne State University, Detroit, Michigan, U.S.A., March 9, 2005.
- 66.\*\* "New Alternatives for Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Diradicals to Excited Electronic States in Molecules and Atomic Nuclei," James Franck Institute, University of Chicago, Chicago, Illinois, U.S.A., March 15, 2005.
- 67.\*\* "New Alternatives for Accurate Quantum Calculations for Molecular Systems: Bond Breaking, Diradicals, and Excited Electronic States," Department of Chemistry, Oakland University, Rochester, Michigan, U.S.A., April 6, 2005.
- 68.\*\* "New Alternatives for Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Diradicals to Excited States in Molecules and Atomic Nuclei," Department of Chemistry and Theoretical Chemistry Institute, University of Wisconsin, Madison, U.S.A., May 9, 2005.
- 69.\*\* "Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Electronic Quasi-Degeneracies and Open-Shell Problems," Fifth Congress of the International Society for Theoretical Chemical Physics (ICTCP-V), New Orleans, Louisiana, U.S.A., July 20-26, 2005.

- 70.\*\* “Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States,” The symposium “Theoretical Determination of Energy Landscapes: Methodology and Applications,” 230th American Chemical Society National Meeting, Washington, DC, U.S.A., August 28-September 1, 2005.
- 71.\*\* “Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Quasi-Degeneracies and Open-Shell Problems,” Conference on Microscopic Approaches to Many-Body Theory, in honor of Professor Raymond Bishop, The University of Manchester, Manchester, U.K., August 31-September 3, 2005.
- 72.\*\* “Active-Space Coupled-Cluster Method: An Inexpensive and Highly Accurate Approach to Electronic Quasi-Degeneracies and Open-Shell Problems,” Tenth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-X, Carthage, Tunisia, September 1-7, 2005.
- 73.\*\* “New Alternatives for Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Biradicals to Excited States in Molecules and Atomic Nuclei,” Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University, Kyoto, Japan, October 6, 2005.
- 74.\*\* “Advances in Electronic Structure Theory: Multi-Reference Coupled-Cluster Methods,” Fukui Institute for Fundamental Chemistry, Kyoto University, Kyoto, Japan, October 31, 2005.
- 75.\*\* “New Alternatives for Accurate Quantum Calculations for Molecular Systems: From Bond Breaking and Biradicals to Excited Electronic States,” Department of Applied Chemistry, School of Engineering, The University of Tokyo, Tokyo, Japan, November 18, 2005.
- 76.\*\* “New Alternatives for Accurate Quantum Calculations for Molecular Systems: From Bond Breaking and Biradicals to Excited Electronic States,” Department of Chemistry, School of Science and Engineering, Waseda University, Tokyo, November 19, 2005.
- 77.\*\* “New Alternatives for Accurate Quantum Calculations for Molecular Systems: From Bond Breaking and Biradicals to Excited Electronic States,” Department of Knowledge-Based Information Engineering, Toyohashi University of Technology, Toyohashi, Japan, November 24, 2005.
- 78.\*\* “New Alternatives for Accurate Quantum Calculations for Molecular Systems: From Bond Breaking and Biradicals to Excited Electronic States,” Department of Chemistry, University of Coimbra, Portugal, March 23, 2006.
- 79.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006.
- 80.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” Unidad Asociada Universidad Autónoma de Madrid – Consejo Superior de Investigaciones Científicas (UAM-CSIC), Instituto de Matemáticas y Física Fundamental, Departamento de Física Atómica, Molecular y de Agregados (Department of Atomic, Molecular, and Cluster Physics), Madrid, Spain, July 14, 2006.

- 81.\*\* “Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Electronic Excitations in Molecules to Properties of Atomic Nuclei,” The Centro Internacional de Matemática Workshop “Mathematics in Chemistry,” Lisbon, Portugal, July 19-21, 2006.
- 82.\*\* “Advances in Electronic Structure Theory: Single-Reference Coupled-Cluster Methods for Multi-Reference Problems,” Sixth Canadian Computational Chemistry Conference (CCCC6), Vancouver, Canada, July 26-30, 2006 [invited plenary lecture].
- 83.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” Eleventh European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XI, St. Petersburg, Russia, August 20-25, 2006.
- 84.\*\* “Accurate Quantum Calculations for Many-Body Systems: From Reaction Mechanisms in Organic and Bioinorganic Chemistries to Properties of Atomic Nuclei,” Michigan State University High Performance Computing Center 2006 Symposium, East Lansing, Michigan, October 7, 2006.
- 85.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” Department of Chemistry, The University of Western Ontario, London, Ontario, Canada, November 8, 2006.
- 86.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” Department of Chemistry, University of Waterloo, Waterloo, Ontario, Canada, November 10, 2006.
- 87.\*\* “Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Properties of Atomic Nuclei,” the S.R. Palit Memorial Lecture, Indian Association for the Cultivation of Science, Kolkata (Calcutta), India, January 9th, 2007.
- 88.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” International Conference “Recent Trends in Many-Body Methods for Electronic Structure and Properties of Atoms and Molecules,” Bhubaneswar and Puri, Orissa, India, January 11-13, 2007.
- 89.\*\* “Active-Space Coupled-Cluster Methods for Bond Breaking, Excited Electronic States, and Open-Shell Systems,” International Conference “Practicing Chemistry with Theoretical Tools, on the Occasion of Professor Mark S. Gordon’s 65th Birthday,” Kihei, Hawaii, U.S.A., January 15-18, 2007.
- 90.\*\* “Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Properties of Atomic Nuclei,” Department of Chemistry, Western Michigan University, Kalamazoo, Michigan, U.S.A., April 2, 2007.
- 91.\*\* “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007.

- 92.\*\* “Coupled-Cluster Theory: An Overview of the Basic Formalism and Applications to Molecular and Nuclear Structure Problems,” Workshop on Advanced Many-body Methods for Nuclear Structure European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 2-6, 2007.
- 93.\*\* “Coupled-Cluster Theory: Basic Formalism, Recent Developments, and Applications to Molecular and Nuclear Structure Problems,” Institut für Kernphysik, Fachbereich Physik, Technische Universität Darmstadt, Darmstadt, Germany, August 29, 2007.
- 94.\*\* “Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, and Bond Breaking,” Twelfth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XII, London, U.K., August 30 - September 5, 2007.
- 95.\*\* “Coupled-Cluster Theory: Basic Formalism, Recent Developments, and Applications to Molecular and Nuclear Structure Problems,” Department of Chemistry, University of Wrocław, Wrocław, Poland, September 10, 2007.
- 96.\*\* “Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, Reaction Pathways, and Photochemistry,” “IXth International Conference on Molecular Spectroscopy: From Molecules to Molecular Biological Systems and Molecular Materials, Role of Molecular Interactions and Recognition,” Wrocław – Łądek-Zdrój, Poland, September 13-18, 2007.
- 97.\*\* “Coupled-Cluster Theory: Basic Formalism, Recent Developments, and Applications to Molecular and Nuclear Structure Problems,” Department of Chemistry, Wake Forest University, Winston-Salem, North Carolina, November 28, 2007.
- 98.\*\* “Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Properties of Atomic Nuclei,” the Computational Materials Seminar Series, Department of Chemistry and Chemical Biology, Cornell University, Ithaca, New York, February 7, 2008.
- 99.\*\* “Coupled-Cluster Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Atomic Nuclei,” Department of Chemistry, University of Michigan, Ann Arbor, Michigan, March 20, 2008.
- 100.\*\* “Coupled-Cluster Calculations for Many-Electron and Other Many-Fermion Systems: From Reaction Pathways in Chemistry to Atomic Nuclei,” Chemistry and Physics Colloquium, Michigan Technological University, Houghton, Michigan, March 27, 2008.
- 101.\*\* “Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell Systems,” The symposium “Electronic Structure and Reaction Dynamics of Open-shell Species,” 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., April 6-10, 2008.
- 102.\*\* “Renormalized Coupled-Cluster Methods: Theoretical Foundations and Molecular Applications,” Center for Computational Chemistry, University of Georgia, Athens, Georgia, May 6, 2008.

- 103.\*\* "Some Developments in Multi-Reference Coupled-Cluster Theory and Applications of Coupled-Cluster Methods to Atomic Nuclei," Center for Computational Chemistry, University of Georgia, Athens, Georgia, May 7, 2008.
- 104.\*\* "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," Sixth Congress of the International Society for Theoretical Chemical Physics (ICTCP-VI), Vancouver, British Columbia, Canada, July 19-24, 2008 [invited plenary lecture].
- 105.\*\* "Coupled-Cluster Theory: A Brief Overview of Modern Methods and Applications to Nuclear Structure," the WE-Heraeus-Seminar "Ab-Initio Nuclear Structure - Where do we stand?", Bad Honnef, Germany, July 28-30, 2008.
- 106.\*\* "Coupled-Cluster Theory: An Overview of Modern Methods and Applications to Nuclear and Electronic Structure," Institut für Kernphysik, Fachbereich Physik, Technische Universität Darmstadt, Darmstadt, Germany, August 4, 2008.
- 107.\*\* "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008.
- 108.\*\* "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," The International Conference on the Theory and Applications of Computational Chemistry in 2008 (TACC 2008), Shanghai, China, September 23-27, 2008 [invited plenary lecture].
- 109.\*\* "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," The symposium "Advances in Electronic Structure Theory and First Principles Dynamics," 237th American Chemical Society National Meeting, Salt Lake City, Utah, U.S.A., March 22-26, 2009.
- 110.\*\* "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States," 30th Annual Combustion Research Meeting, Airlie Conference Center, Warrenton, Virginia, May 26-29, 2009.
- 111.\*\* "Coupled-Cluster Theory: From Quantum Chemistry to Applications in Nuclear Physics," International Workshop "Linking Nuclei, Molecules, and Condensed Matter: Computational Quantum Many-Body Approaches," European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 6-10, 2009.
- 112.\*\* "Dealing with Strong Electron Correlations in Quantum Chemistry via Renormalized, Active-Space, and Multi-Reference Coupled-Cluster Methods," The symposium "New Developments in Strongly Correlated Electrons," 238th American Chemical Society National Meeting, Washington, DC, U.S.A., August 16-20, 2009.
- 113.\*\* "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," Fourteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XIV, San Lorenzo del Escorial, Madrid, Spain, September 13-19, 2009.

- 114.\*\* TBA, Department of Chemistry, Iowa State University, Ames, Iowa, U.S.A., October 2, 2009.
- 115.\*\* TBA, International conference on “Recent Advances in Many-Electron Theories,” Raman Center for the Atomic, Molecular, and Optical Sciences, Indian Association for the Cultivation of Science, Kolkata, India, January 4-6, 2010.
- 116.\*\* TBA, 10-minute perspective talk preceding a session on multi-reference coupled-cluster theory, the 50th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 24-March 2, 2010.
- 117.\*\* TBA, International conference “Molecular Quantum Mechanics: From Methylene to DNA and Beyond” honoring Professor Henry F. Schaefer’s work, University of California at Berkeley, Berkeley, California, May 24-29, 2010.

In addition, Dr. Piotr Piecuch has been invited to present a paper “New Coupled-Cluster Methods for Molecular Potential Energy Surfaces” at the 262nd WE-Heraeus-Seminar entitled “Modern Aspects of Many-Electron Theory,” Bad Honnef, Germany, October 21–24, 2001 [classified as invited poster].

## LIST OF PAPERS PRESENTED AT CONFERENCES<sup>†</sup>

1. P. Piecuch, "Invariance Properties of the Multipole Expansion," The Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Lublin, Poland, September 22-25, 1982 [oral presentation].
2. P. Piecuch, "Spherical Tensor Operators in Theory of Long-Range Intermolecular Interactions," The Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Lublin, Poland, September 22-25, 1982 [oral presentation].
3. P. Piecuch, "Spherical Tensor Theory of Long-Range Intermolecular Forces Including Quantum-Mechanical Many-Body Effects," Fourth School of Advanced Methods of Quantum Chemistry, Bachotek, Poland, May 27-31, 1985 [poster presentation].
4. P. Piecuch, "Simple Derivation of the Multipole Expansion in the Spherical Tensor Form. The Use of Stone's Cartesian-Spherical Transformation Formalism," Fourth School of Advanced Methods of Quantum Chemistry, Bachotek, Poland, May 27-31, 1985 [poster presentation].
5. P. Piecuch, "Mathematical Apparatus of the Quantum Theory of Angular Momentum and the Formalism of Irreducible Tensor Operators in the Perturbation Theory of Long-Range Interactions between  $N$  Molecules Including Many-Body Effects," Microsymposium of the Quantum Chemistry Section of the Polish Chemical Society organized during the Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Poznań, Poland, September 4-7, 1985 [poster presentation].
6. P. Piecuch, "Magnitudes of Higher-Order Interaction Energy Contributions Appearing in the Perturbative Description of Long-Range Intermolecular Interactions. Interactions in the Typical Simple Molecular Complexes  $H_2 - He$  and  $H_2 - H_2$ ," Microsymposium of the Quantum Chemistry Section of the Polish Chemical Society organized during the Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Poznań, Poland, September 4-7, 1985 [poster presentation].
7. P. Piecuch, "Anisotropic and Isotropic Two- and Many-Body Long-Range Intermolecular Interactions – the Use of Racah-Wigner Algebra and the Formalism of Irreducible Tensors," Conference "The Nature of Molecular Interactions," Karpacz, Poland, June 8-12, 1986 [poster presentation].
8. P. Piecuch, "Spherical Tensor Theory of Long-Range Molecular Interactions Including Quantum-Mechanical Many-Body Effects," International Symposium "Molecules in Physics, Chemistry and Biology," Paris, France, June 15-21, 1986 [poster presentation].

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<sup>†</sup> Presentations of results that have been obtained at Michigan State University before submitting the tenure promotion package in the Fall of 2001 are marked by \*. Presentations given after submitting the tenure promotion package in the Fall of 2001 are marked by \*\*.

9. P. Piecuch, "Classification and Mathematical Description of Two- and Many-Body Long-Range Interactions in a System of  $N$  Arbitrary Molecules," Conference "Quantum Chemistry - 86," Wrocław, Poland, December 5-6, 1986 [oral presentation].
10. P. Piecuch, "Theoretical Insight into Many-Body Long-Range Effects of the Electrostatic Origin in Multimolecular Systems," 35. Bunsen-Kolloquium "Interactions of Water in Ionic and Nonionic Hydrates," Marburg, April 2-3, 1987 (and subsequent seminar of the Department of Physical Chemistry of the University of Marburg, April 4, 1987), Federal Republic of Germany [poster presentation].
11. P. Piecuch, "Elementary Derivation of the Addition Theorems for Solid Spherical Harmonics," Second School "Current Trends in Theoretical Chemistry," Zakopane, Poland, May 27-31, 1987 [poster presentation].
12. P. Piecuch, "Spherical Tensor Theory of Long-Range Intermolecular Forces Including Quantum-Mechanical Many-Body Effects: the Use of Cartesian-Spherical Transformation Formalism," Fifth School of Advanced Methods of Quantum Chemistry "Bachotek '87," Bachotek, Poland, May 31-June 5, 1987 [poster presentation].
13. P. Piecuch, "Analytical Description of Two- and Many-Body Fourth-Order Induction Interaction Energies in Multimolecular Systems within Spherical Tensor Formalism," Eighth International Symposium on Solute-Solute-Solvent Interactions, Regensburg, Federal Republic of Germany, August 9-14, 1987 [oral presentation].
14. P. Piecuch, "Classification and Analytical Description of Two- and Many-Body Fourth-Order Induction Interaction Energies in Multimolecular Systems within Spherical Tensor Formalism," VIII-th Workshop "Horizons in Hydrogen Bond Research," Polanica Zdrój near Wrocław, Poland, September 10-16, 1987 [poster presentation].
15. P. Piecuch, "Generalization of the Concept of Spherical Harmonic Expansions to Many-Body Intermolecular Forces. Application to the Case of Fourth-Order Induction Interactions in an Arbitrary Multimolecular System," Regional Symposium on Chemical Physics, University of Waterloo, Waterloo, Ontario, Canada, October 28-30, 1988 [poster presentation].
16. P. Piecuch and J. Paldus, "Orthogonally Spin-Adapted Coupled-Cluster Equations. Comparison of Different Procedures for Spin-Adaptation," Regional Symposium on Chemical Physics, University of Waterloo, Waterloo, Ontario, Canada, October 28-30, 1988 [poster presentation].
17. P. Piecuch, S. Zarrabian, J. Paldus, and J. Čížek, "Coupled-Cluster Approach with Approximate Account of Triple Excitations and its Application to the Cyclic Polyene Model Systems," 10th Canadian Symposium on Theoretical Chemistry, Banff, Alberta, Canada, August 24-30, 1989 [poster presentation].
18. P. Piecuch, S. Zarrabian, J. Paldus, and J. Čížek, "Limitations in Determining the Lower Bounds to the Ground State Correlation Energy of the Cyclic Polyenes Using Optimized Inner Projection Technique," 10th Canadian Symposium on Theoretical Chemistry, Banff, Alberta, Canada, August 24-30, 1989 [poster presentation].

19. P. Piecuch, S. Zarrabian, J. Paldus, and J. Čížek, "Account of Higher than Pair Cluster Contributions in Single Reference Coupled Cluster Theory," The 6<sup>th</sup> Annual University of Waterloo Symposium on Chemical Physics, University of Waterloo, Waterloo, Ontario, Canada, October 26-28, 1990 [poster presentation].
20. P. Piecuch and J. Paldus, "Orthogonally Spin-Adapted Multi-Reference Coupled-Cluster Formalism. Comparison of Different Procedures for Spin-Adaptation," 1991 Sanibel Symposia on Atomic, Molecular, and Condensed Matter Theory, Computational Methods, and the Application of Fundamental Theory to Problems of Biology and Pharmacology, St. Augustine, Florida, U.S.A., March 9-16, 1991 [poster presentation].
21. J. Paldus, P. Piecuch, B. Jeziorski, and L. Pylypow, "Extension of Coupled Cluster Methodology to Open Shells: State-Universal Approach," Seventh International Conference on Recent Progress in Many-Body Theories, Minneapolis, Minnesota, U.S.A., August 26-31, 1991 [invited talk given by J. Paldus].
22. P. Piecuch, R. Tobała, J. Paldus, and H. Chojnacki, "Approximate Method of Accounting for Quadruple Excitations in Multi-Reference Coupled-Cluster Theory. Application to H<sub>4</sub> Model System," Quantum Chemistry Symposium on Methods and Applications of Quantum Chemistry in Studies of Molecular Systems organized by the Institute of Chemistry of the Silesian University in cooperation with Quantum Chemistry Section of the Polish Chemical Society, Katowice, Poland, September 18, 1992 [poster presentation].
23. P. Piecuch, "Application of the Hilbert-Space Coupled-Cluster Theory to Electronic States of the H<sub>4</sub> Model System," Workshop "Coupled Clusters in the Theory of Atoms and Molecules," Quantum Chemistry Laboratory, Faculty of Chemistry, University of Warsaw, Poland, October 23-24, 1992 [invited talk].
24. J. Paldus, X. Li, and P. Piecuch, "Degeneracy and Coupled-Cluster Methods ('Variations on a Theme')," 1993 Sanibel Symposia on Atomic, Molecular, and Condensed Matter Theory, Computational Methods, and the Application of Fundamental Theory to Problems of Biology and Pharmacology, St. Augustine, Florida, U.S.A., March 13-20, 1993 [poster presentation].
25. J. Paldus and P. Piecuch, "Exclusion Principle Violating (EPV) Diagrams: A Mathematical Convenience or a Physically Important Concept?," 5th International Conference on Mathematical and Computational Chemistry, University of Missouri-Kansas City, Kansas City, Missouri, U.S.A., May 17-21, 1993 [talk given by J. Paldus].
26. P. Piecuch and L. Adamowicz, "A State-Selective Multi-Reference Coupled-Cluster Method Employing the Single-Reference Formalism: Theory, Implementation and a Test Case Study," 14th Annual West Coast Theoretical Chemistry/Statistical Mechanics Conference, University of California, Los Angeles, California, U.S.A., June 17-19, 1993 [contributed talk given by P. Piecuch].
27. P. Piecuch and L. Adamowicz, "A State-Selective Multi-Reference Coupled-Cluster Method Employing the Single-Reference Formalism: Theory, Implementation and a Model Study," Eighth American Conference on Theoretical Chemistry, University of Rochester, Rochester, New York, U.S.A., June 27-July 2, 1993 [poster presentation].

28. P. Piecuch and L. Adamowicz, "Breaking Bonds with the SS MRCC Method," 15th Annual West Coast Theoretical Chemistry/Statistical Mechanics Conference, Sandia National Laboratories, Livermore, California, U.S.A., April 27-29, 1994 [poster presentation].
29. V. Alexandrov, P. Piecuch, and L. Adamowicz, "State-Selective Multireference Coupled-Cluster Theory Employing Single-Reference Formalism: Implementation and Application to Excited States of LiH and H<sub>8</sub>," 15th Annual West Coast Theoretical Chemistry/Statistical Mechanics Conference, Sandia National Laboratories, Livermore, California, U.S.A., April 27-29, 1994 [contributed talk given by V. Alexandrov].
30. P. Piecuch and J. Paldus, "Orthogonally Spin-Adapted Hilbert-Space Coupled-Cluster Formalism. Importance of the High-Order Coupling Terms," Second Canadian Computational Chemistry Conference, Queen's University at Kingston, Kingston, Ontario, Canada, May 21-25, 1994 [plenary talk given by P. Piecuch].
31. P. Piecuch, V. Alexandrov, and L. Adamowicz, "A State-Selective Multi-Reference Coupled-Cluster Method Employing the Single-Reference Formalism: Theory, Implementation and a Model Study," 8th International Congress of Quantum Chemistry, Satellite Meeting "Electron Correlation in Atoms and Molecules; New Methods and Applications," Smolenice Castle near Bratislava, Slovak Republic, June 14-18, 1994 [talk given by L. Adamowicz].
32. R. Tobiła, P. Piecuch, and J. Paldus, "Coupled Cluster Approaches with an Approximate Account of Triply and Quadruply Excited Clusters: Implementation of the Orthogonally Spin-Adapted CCD+ST(CCD), CCSD+T(CCSD) and ACPQ+ST(ACPQ) Formalisms," 8th International Congress of Quantum Chemistry, Satellite Meeting "Electron Correlation in Atoms and Molecules; New Methods and Applications," Smolenice Castle near Bratislava, Slovak Republic, June 14-18, 1994 [poster presentation].
33. R. Tobiła, P. Piecuch, J. Paldus, and H. Chojnacki, "Coupled Cluster Approaches with an Approximate Account of Triply and Quadruply Excited Clusters: Implementation of the Orthogonally Spin-Adapted CCD+ST(CCD) and ACPQ+ST(ACPQ) Formalisms," The Scientific Convention of the Polish Chemical Society and of the Association of Chemical Industry Engineers and Technicians, Warsaw, Poland, September 12-15, 1994 [poster presentation].
34. P. Piecuch and J. Paldus, "Coupled-Cluster Methods for Quasidegenerate States. Calculation of Potential Energy Surfaces and Molecular Properties Using the State-Universal Multi-Reference Coupled-Cluster Approach," The 10<sup>th</sup> Annual University of Waterloo Symposium on Chemical Physics, University of Waterloo, Waterloo, Ontario, Canada, November 4-6, 1994 [plenary talk given by P. Piecuch].
35. A.E. Kondo, P. Piecuch, and J. Paldus, "Orthogonally Spin-Adapted Single-Reference Coupled-Cluster Formalism: Linear Response Calculation of Static Properties," The 10<sup>th</sup> Annual University of Waterloo Symposium on Chemical Physics, University of Waterloo, Waterloo, Ontario, Canada, November 4-6, 1994 [poster presentation].
36. P. Piecuch, A.E. Kondo, V. Špirko, and J. Paldus, "Calculation of Property Functions Using the Single- and Multi-Reference Coupled-Cluster Approaches," 12th Canadian

Symposium on Theoretical Chemistry, Fredericton, New Brunswick, Canada, August 6-11, 1995 [poster presentation].

37. J. Paldus, X. Li, and P. Piecuch, "Recent Developments in Coupled-Cluster Theory," 1995 International Chemical Congress of Pacific Basin Societies (PACIFICHEM '95), Honolulu, Hawaii, U.S.A., December 17-22, 1995 [invited talk given by J. Paldus].
38. J. Paldus, P. Piecuch, X. Li, and A.E. Kondo, "Coupled Cluster Approach to Static Properties," Canadian Society for Chemistry, 79th Conference and Exhibition, Memorial University of Newfoundland, St. John's, Canada, June 23-26, 1996 [invited talk given by J. Paldus].
39. P. Piecuch, A.E. Kondo, J. Paldus, and V. Špirko, "Linear Response Coupled-Cluster Approach to Static Molecular Properties," The symposium "Frontiers in Electronic Structure Theory," 213th American Chemical Society National Meeting, San Francisco, California, U.S.A., April 13-17, 1997 [invited talk given by P. Piecuch].
40. P. Piecuch, "Coupled-Cluster Approach to Static Molecular Properties," Workshop "Coupled Cluster Theory and Electron Correlation, Fifty Years of the Correlation Problem," Cedar Key, Florida, U.S.A., June 15-19, 1997, a satellite meeting of the 9th International Congress of Quantum Chemistry, Atlanta, Georgia, U.S.A., June 9-14, 1997 [invited talk].
41. M.S. Topaler, D.G. Truhlar, X.Y. Chang, P. Piecuch, and J.C. Polanyi, "Fit of Potential Energy Surfaces and Theoretical Study of NaFH Absorption and Photodissociation Cross Sections," 1997 Conference on the Dynamics of Molecular Collisions, Gull Lake, Minnesota, U.S.A., July 21-25, 1997 [poster presentation].
42. P. Piecuch and R.J. Bartlett, "EOMXCC: A New Coupled-Cluster Method for Electronically Excited States," Thirty-Eighth Sanibel Symposium on Atomic, Molecular, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 21-27, 1998 [poster presentation].
43. P. Piecuch, S.A. Kucharski, and R.J. Bartlett, "Coupled-Cluster Methods with Internal and Semi-Internal Triply and Quadruply Excited Clusters: CCSDt and CCSDtq Approaches," Twenty-Seventh Southeastern Theoretical Chemistry Association Conference, Tallahassee, Florida, U.S.A., May 28-30, 1998 [contributed talk given by P. Piecuch].
- 44.\* V. Špirko, P. Piecuch, and O. Bludsky, "Quasi-Bound States of the Na $\cdots$ FH van der Waals Molecule," Thirty-Ninth Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 27-March 5, 1999 [poster presentation].
- 45.\* S.A. Kucharski, P. Piecuch, and R.J. Bartlett, "Potential Energy Curves for the N<sub>2</sub> Molecule: A Coupled Cluster Study Including Connected Quadruply Excited Clusters," Thirty-Ninth Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 27-March 5, 1999 [poster presentation].

- 46.\* P. Piecuch, "Single-Reference Coupled-Cluster Methods for Quasi-Degenerate Electronic States," The symposium "Electronic Structure Theory: From Methods to Molecules and Materials," 100th Annual Meeting of the American Physical Society, Atlanta, Georgia, U.S.A., March 21-26, 1999 [invited talk].
- 47.\* J.B. Giorgi, T.G. Lee, A.J. Hudson, F. Naumkin, H.-B. Oh, P. Piecuch, and J.C. Polanyi, "Harpooning Studied by Transition-State Spectroscopy:  $M \cdot XR + h\nu \rightarrow [M^* \cdot XR]^\ddagger \rightarrow [M^+ \cdot \cdot \cdot XR^-]^\ddagger \rightarrow$  products ( $X = F, Cl, Br$ ;  $R = H, CH_3$ )," The symposium "Electronically Nonadiabatic Processes in Gaseous, Cluster, and Condensed Media," 218th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., August 22-26, 1999 [invited talk given by J.C. Polanyi].
- 48.\* P. Piecuch, "Dynamics of Harpooning in van der Waals Molecules," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [invited talk].
- 49.\* K. Kowalski and P. Piecuch, "On the Origin of Intruder State Problem in Multi-Reference Coupled-Cluster Theory," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [poster presentation].
- 50.\* K. Kowalski, P. Piecuch, and K. Jankowski, "A Complete Set of Solutions of Coupled-Cluster Equations Involving Triply and Quadruply Excited Clusters," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [poster presentation].
- 51.\* P. Piecuch and J.I. Landman, "Parallelization of Multi-Reference Coupled-Cluster Method," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [poster presentation].
- 52.\* P. Piecuch, S.A. Kucharski, and V. Špirko, "Coupled-Cluster Methods with Internal and Semi-Internal Triply Excited Clusters: Vibrational Spectrum of the HF Molecule," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [poster presentation].
- 53.\* R.J. Bartlett, S.A. Kucharski, P. Piecuch, K. Wilson, M. Kolaski, and S.A. Perera, "Coupled-Cluster Theory: Recent Progress," The symposium "11th European Seminar on Computational Methods in Quantum Chemistry," Zakopane, Poland, September 23-25, 1999 [invited talk given by R.J. Bartlett].
- 54.\* P. Piecuch, "Dynamics of Harpooning in van der Waals Molecules," "Vth International Conference on Molecular Spectroscopy," Łądek-Zdrój, Poland, September 26-30, 1999 [invited talk].
- 55.\* P. Piecuch and K. Kowalski, "Method of Moments of Coupled Cluster Equations: A New Approach to the Many-Electron Correlation Problem," 40th Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 26-March 3, 2000 [poster presentation].

- 56.\* K. Kowalski and P. Piecuch, "The Complete Sets of Solutions of the Bloch and State-Universal Multi-Reference Coupled-Cluster Equations," 40th Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 26-March 3, 2000 [poster presentation].
- 57.\* R. Burcl, P. Piecuch, V. Špirko, and O. Bludský, "Bound and Quasi-Bound States of the  $\text{Li} \cdots \text{FH}$  van der Waals Molecule," 40th Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 26-March 3, 2000 [poster presentation].
- 58.\* J.B. Giorgi, T.G. Lee, A.J. Hudson, F. Naumkin, H.-B. Oh, P. Piecuch, and J.C. Polanyi, "Harpooning Studied by Transition-State Spectroscopy:  $\text{M} \cdots \text{XR} + h\nu \rightarrow [\text{M}^* \cdots \text{XR}]^\ddagger \rightarrow [\text{M}^+ \cdots \text{XR}^-]^\ddagger \rightarrow \text{products}$ : Results for  $\text{M} = \text{Li}$ ,  $\text{X} = \text{F}$ ,  $\text{R} = \text{H}, \text{CH}_3$ ," The symposium "Computers in Chemistry Award Symposium Honoring Don Truhlar," 219th American Chemical Society National Meeting, San Francisco, California, U.S.A., March 26-30, 2000 [invited talk given by J.C. Polanyi].
- 59.\* P. Piecuch and K. Kowalski, "Method of Moments of Coupled-Cluster Equations: A New Approach to the Many-Electron Correlation Problem," The 2000 Florida Award Symposium (honoring Dr. Rodney J. Bartlett's work), FAME 2000 (Florida Annual Meeting and Exposition, organized by the Florida Section of the American Chemical Society), Orlando, Florida, U.S.A., May 12, 2000 [invited talk given by P. Piecuch].
- 60.\* P. Piecuch, "Dynamics of Photo-Induced Charge Transfer in van der Waals Molecules," Joint Polish-German Conference on Modern Optics: Fundamental Aspects of Spectroscopy and Environmental Applications, Jurata near Gdańsk, Poland, September 17-22, 2000 [invited talk].
- 61.\* R. Burcl, P. Piecuch, V. Špirko, and O. Bludsky, "Bound and Quasi-Bound States of the  $\text{Li} \cdots \text{FH}$  van der Waals Molecule," The 16th Annual Symposium on Chemical Physics at the University of Waterloo, Waterloo, Ontario, Canada, November 3-5, 2000 [contributed talk, given by R. Burcl].
- 62.\* E. Kratz, R. Burcl, P. Piecuch, and V. Špirko, "*Ab Initio* Studies of the  $\text{Li} \cdots \text{FCH}_3$  van der Waals Complex," The 16th Annual Symposium on Chemical Physics at the University of Waterloo, Waterloo, Ontario, Canada, November 3-5, 2000 [poster presented by R. Burcl].
- 63.\* P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," the 41st Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 24-March 2, 2001 [invited talk].
- 64.\* K. Kowalski and P. Piecuch, "New Equation-of-Motion Coupled-Cluster Methods," the 41st Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 24-March 2, 2001 [poster, presented by K. Kowalski].
- 65.\* P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," First Southern School on Computational Chemistry, Orange Beach, Alabama, March 24, 2001 [invited talk].

- 66.\* P. Piecuch and K. Kowalski, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," 14th Canadian Symposium on Theoretical Chemistry, Carleton University, Ottawa, Canada, August 4–9, 2001 [contributed talk given by P. Piecuch; one of the three posters selected for oral presentations].
- 67.\* P. Piecuch, V. Špirko, R. Burcl, K. Kowalski, S.A. Kucharski, F. Mrugała, and O. Bludsky, "Effect of the Potential Energy Surface on the Dynamics of Weakly Bound Precursor Complexes and New "Black-Blox" Coupled-Cluster Methods for Entire Potential Energy Surfaces of Reactive Molecular Systems," The symposium "First Principles Chemical Reaction Dynamics," 222nd American Chemical Society National Meeting, Chicago, Illinois, U.S.A., August 26–30, 2001 [invited talk given by P. Piecuch].
- 68.\* P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," 34th Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, Minnesota, U.S.A., October 5–6, 2001 [invited talk].
- 69.\* K. Kowalski and P. Piecuch, "New Equation-of-Motion Coupled-Cluster Methods," 34th Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, Minnesota, U.S.A., October 5–6, 2001 [poster presented by K. Kowalski].
- 70.\* A.W. Jasper, M.D. Hack A. Chakraborty, P. Piecuch, and D.G. Truhlar, "Photodissociation of LiFH and NaFH van der Waals Complexes: A Semiclassical Trajectory Study," 34th Midwest Theoretical Chemistry Conference, University of Minnesota, Minneapolis, Minnesota, U.S.A., October 5–6, 2001 [poster presented by A.W. Jasper].
- 71.\* P. Piecuch, K. Kowalski, and I.S.O. Pimienta, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," the 262nd WE-Heraeus-Seminar entitled "Modern Aspects of Many-Electron Theory," Bad Honnef, Germany, October 21–24, 2001 [invited poster, presented by P. Piecuch].
- 72.\*\* K. Kowalski and P. Piecuch, "New Coupled-Cluster Methods for Excited States," 10th Conference on Current Trends in Computational Chemistry, Jackson, Mississippi, U.S.A., November 1–3, 2001 [poster presented by K. Kowalski].
- 73.\*\* P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces: I. Ground-State Approaches," SciDAC Kick-Off Meeting, Reston, Virginia, U.S.A., January 15-16, 2002 [poster].
- 74.\*\* P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces: II. Excited-State Approaches," SciDAC Kick-Off Meeting, Reston, Virginia, U.S.A., January 15-16, 2002 [poster].
- 75.\*\* P. Piecuch, "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Quasi-Degenerate Ground States, Molecular Potential Energy Surfaces, and Excited States," Institute for Nuclear Theory workshop on "Advanced Computational Methods for Solving the Nuclear Many-Body Problem," Seattle, Washington, U.S.A., March 12–15, 2002 [invited talk].
- 76.\*\* P. Piecuch, K. Kowalski, and I.S.O. Pimienta, "New Single- and Multi-Reference Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," The

- symposium "Recent Advances in Electron Correlation Methodology," 223rd American Chemical Society National Meeting, Orlando, Florida, U.S.A., April 7–11, 2002 [invited talk given by P. Piecuch].
- 77.\*\* P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces: Recent Progress and Milestones," BES SciDAC PI Workshop, Argonne National Laboratory, Argonne, Illinois, U.S.A., June 13-14, 2002 [poster].
- 78.\*\* I.S.O. Pimienta, K. Kowalski, and P. Piecuch, "Method of Moments of Coupled-Cluster Equations: Inclusion of All Generalized Moments of the Coupled-Cluster Singles and Doubles Equations," The 2002 American Conference on Theoretical Chemistry, Seven Springs Mountain Resort, Champion, Pennsylvania, U.S.A., July 13-18, 2002 [poster presented by I.S.O. Pimienta].
- 79.\*\* K. Kowalski and P. Piecuch, "New Equation-of-Motion Coupled-Cluster Methods," The 2002 American Conference on Theoretical Chemistry, Seven Springs Mountain Resort, Champion, Pennsylvania, U.S.A., July 13-18, 2002 [poster presented by K. Kowalski].
- 80.\*\* M.J. McGuire, E. Kratz, R. Burcl, and P. Piecuch, "The Unusual Effect of the Basis Set Superposition Error on the Geometries and Bending Potentials of the  $\text{Li} \cdots \text{FCH}_3$  and  $\text{Na} \cdots \text{FCH}_3$  Complexes," The 2002 American Conference on Theoretical Chemistry, Seven Springs Mountain Resort, Champion, Pennsylvania, U.S.A., July 13-18, 2002 [poster presented by M.J. McGuire].
- 81.\*\* M.J. McGuire, K. Kowalski, and P. Piecuch, "Renormalized Coupled-Cluster Calculations of Reactive Potential Energy Surfaces: The Collinear BeFH System," The 2002 American Conference on Theoretical Chemistry, Seven Springs Mountain Resort, Champion, Pennsylvania, U.S.A., July 13-18, 2002 [poster presented by M.J. McGuire].
- 82.\*\* P.-D. Fan, K. Jedziniak, K. Kowalski, and P. Piecuch, "On the Exactness of Two-Body Cluster Expansions in Many-Body Quantum Theory," The 2002 American Conference on Theoretical Chemistry, Seven Springs Mountain Resort, Champion, Pennsylvania, U.S.A., July 13-18, 2002 [poster presented by P.-D. Fan].
- 83.\*\* P. Piecuch, K. Kowalski, I.S.O. Pimienta, and M.J. McGuire, "Method of Moments of Coupled-Cluster Equations: A New Framework for Designing Accurate Electronic Structure Methods," Fourth International Congress of the International Society for Theoretical Chemical Physics (ICTCP-IV), Marly-le-Roi near Paris, France, July 9-16, 2002 [invited plenary talk given by P. Piecuch].
- 84.\*\* P. Piecuch, "Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate Electronic Structure Methods," International Symposium on Frontiers in Molecular Science 2002, Qingdao, China, July 15-18, 2002 [invited talk].
- 85.\*\* P. Piecuch, K. Kowalski, and I.S.O. Pimienta, "Advances in Electronic Structure Theory: New Coupled-Cluster Methods for Molecular Potential Energy Surfaces and Excited States," 6th World Congress of Theoretically Oriented Chemists (WATOC02), Lugano, Switzerland, August 4-9, 2002 [contributed talk; paper selected by the Organizers for the oral presentation].

- 86.\*\* P. Piecuch, K. Kowalski, I.S.O. Pimienta, M.J. McGuire, and P.-D. Fan, "Method of Moments of Coupled-Cluster Equations: A New Theoretical Framework for Designing Highly Accurate (Virtually Exact) and Inexpensive Electronic Structure Methods," 11th Conference on Current Trends in Computational Chemistry, Jackson, Mississippi, U.S.A., November 1-2, 2002 [invited talk given by P. Piecuch].
- 87.\*\* I.S.O. Pimienta, P. Piecuch, and K. Kowalski, "Method of Moments of Coupled-Cluster Equations: Inclusion of All Generalized Moments of the Coupled-Cluster Singles and Doubles Equations," the 43rd Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 22-March 1, 2003 [poster, presented by I.S.O. Pimienta].
- 88.\*\* P.-D. Fan, K. Kowalski, and P. Piecuch, "New Alternatives for Electronic Structure Theory: The Applications of Two-Body Cluster Expansions in Accurate *Ab Initio* Calculations," the 43rd Sanibel Symposium on Atomic, Molecular, Biophysical, and Condensed Matter Theory, St. Augustine, Florida, U.S.A., February 22-March 1, 2003 [poster, presented by P.-D. Fan].
- 89.\*\* P. Piecuch, "New Coupled-Cluster Methods for Molecular Potential Energy Surfaces," 2003 DOE SciDAC PI Meeting, Napa, California, U.S.A., March 10-11, 2003 [poster].
- 90.\*\* P. Piecuch, K. Kowalski, I.S.O. Pimienta, and P.-D. Fan, "New Alternatives for Accurate Electronic Structure Calculations of Molecular Potential Energy Surfaces," The symposium "New Electronic Structure Methods: From Molecules to Materials," 225th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., March 23-27, 2003 [invited talk given by P. Piecuch].
- 91.\*\* P. Piecuch, K. Kowalski, P.-D. Fan, and K. Jedziniak, "On the Exactness of Two-Body Cluster Expansions in Many-Body Quantum Theory," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [talk given by P. Piecuch].
- 92.\*\* K. Kowalski and P. Piecuch, "A New Class of Noniterative Energy Corrections to Coupled-Cluster Energies for Excited Electronic States," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [talk given by K. Kowalski].
- 93.\*\* M.J. McGuire, P. Piecuch, K. Kowalski, S.A. Kucharski, and M. Musiał, "Renormalized Coupled-Cluster Calculations of Reactive Potential Energy Surfaces: A Comparison of the CCSD(T), Renormalized CCSD(T), and Multi-Reference Configuration Interaction Results for the BeFH System," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [poster presented by M.J. McGuire].
- 94.\*\* M.J. McGuire, E. Kratz, R. Burcl, and P. Piecuch, "The Unusual Effect of the Basis Set Superposition Error on the Geometries and Bending Potentials of the  $\text{Li} \cdots \text{FCH}_3$  and  $\text{Na} \cdots \text{FC H}_3$  Complexes," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12-14, 2003 [talk given by M.J. McGuire].

- 95.\*\* I.S.O. Pimienta, Piotr Piecuch, and K. Kowalski, "Method of Moments of Coupled-Cluster Equations: Inclusion of All Generalized Moments of the Coupled-Cluster Singles and Doubles Equations," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12–14, 2003 [talk given by I.S.O. Pimienta].
- 96.\*\* P.-D. Fan, K. Kowalski, and P. Piecuch, "The Application of the Extended Coupled-Cluster Method with Singles and Doubles in Studies of Bond Breaking," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12–14, 2003 [talk given by P.-D. Fan].
- 97.\*\* M. Lodrigo, P.-D. Fan, K. Kowalski, and P. Piecuch, "Method of Moments of Coupled-Cluster Equations Employing the Extended Coupled-Cluster Theory: Dissociation of the N<sub>2</sub> Triple Bond," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12–14, 2003 [poster presented by M. Lodrigo].
- 98.\*\* R.C. Lafuente, P. Piecuch, and K.L.C. Hunt, "Towards the Development and Implementation of Computer Programs for Calculating the Charge-Density Susceptibility," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12–14, 2003 [poster presented by R.C. Lafuente].
- 99.\*\* R.M. Olson, S.A. Varganov, M.S. Gordon, G. Mill, H. Metiu, and P. Piecuch, "2D/3D Transition of Small Gold Clusters (Au<sub>n</sub>|n = 4, 6, 8, ...)," 35th Midwest Theoretical Chemistry Conference, Iowa State University, Ames, Iowa, U.S.A., June 12–14, 2003 [poster presented by R.M. Olson].
- 100.\*\* P. Piecuch, K. Kowalski, I.S.O. Pimienta, P.-D. Fan, and M.J. McGuire, "Single- and Multi-reference Coupled-Cluster Methods for Quasidegenerate Electronic States and Bond Breaking," The symposium "Bond-Breaking Methods in Gas and Condensed Phases," 226th American Chemical Society National Meeting, New York, New York, U.S.A., September 7-11, 2003 [invited talk given by P. Piecuch].
- 101.\*\* K. Kowalski and P. Piecuch, "A New Class of Noniterative Energy Corrections to Coupled-Cluster Energies for Excited Electronic States," The symposium "Bond-Breaking Methods in Gas and Condensed Phases," 226th American Chemical Society National Meeting, New York, New York, U.S.A., September 7-11, 2003 [talk given by K. Kowalski].
- 102.\*\* T. Kuś, S.A. Kucharski, M.J. McGuire, K. Kowalski, and P. Piecuch, "Potential Energy Curves of Open-Shell Systems Obtained with Coupled-Cluster Methods with the T<sub>3</sub> Operator," The 46th Meeting of the Polish Chemical Society, Lublin, Poland, September 15-19, 2003 [poster presented by T. Kuś].
- 103.\*\* P.-D. Fan, K. Kowalski, M. Lodrigo, and P. Piecuch, "New Alternatives for Accurate *Ab Initio* Calculations," 12th Conference on Current Trends in Computational Chemistry, Jackson, Mississippi, U.S.A., October 31-November 1, 2003 [poster presented by P.-D. Fan].
- 104.\*\* P. Piecuch, "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States," 2004 DOE SciDAC PI Meeting, Charleston, South Carolina, U.S.A., March 22-24, 2004 [poster].

- 105.\*\* P. Piecuch and K. Kowalski, "Noniterative Coupled-Cluster Methods for Accurate Calculations of Excited Electronic States," The symposium "The Systematic Treatment of Electron Correlation. A Celebration of the Science of Rodney J. Bartlett," St. Simons Island, Georgia, U.S.A., April 23-25, 2004 [invited talk given by P. Piecuch].
- 106.\*\* D.J. Dean, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, and P. Piecuch, "Coupled-Cluster Approaches to Nuclei, Ground States and Excited States," 8th International Spring Seminar on Nuclear Physics, Key Topics in Nuclear Structure, Paestum, Italy, May 23-27, 2004 [invited talk given by M. Hjorth-Jensen].
- 107.\*\* P.-D. Fan, K. Kowalski, and P. Piecuch, "Intriguing Accuracy of Two-Body Cluster Expansions of Ground and Excited States," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by P.-D. Fan].
- 108.\*\* K. Kowalski and P. Piecuch, "New Classes of Noniterative Energy Corrections to Multireference Coupled-Cluster Energies," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by K. Kowalski].
- 109.\*\* R.C. Lafuente, K.L.C. Hunt, and P. Piecuch, "Preliminary Development and Implementation of Computer Programs for Calculating the Charge-Density Susceptibility," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by R.C. Lafuente].
- 110.\*\* M. Lodriguito, K. Kowalski, and P. Piecuch, "Method of Moments of Coupled-Cluster Equations Employing the Multireference Perturbation Theory," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by M. Lodriguito].
- 111.\*\* M.J. McGuire and P. Piecuch, "Application of Renormalized Coupled-Cluster Methods to Reactions Involving Diradicals," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by M.J. McGuire].
- 112.\*\* K. Kowalski, M. Włoch, and P. Piecuch, "Efficient Implementation of the Standard and Renormalized Equation-of-Motion Coupled-Cluster Methods in GAMESS," 36th Midwest Theoretical Chemistry Conference, Michigan State University, East Lansing, Michigan, U.S.A., June 17-19, 2004 [poster presented by M. Włoch].
- 113.\*\* D.J. Dean, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, and P. Piecuch, "Coupled-Cluster Approaches to Nuclei, Ground States and Excited States," International Nuclear Physics Conference, INPC 2004, Göteborg, Sweden, June 27-July 2, 2004 [invited talk given by M. Hjorth-Jensen].
- 114.\*\* P. Piecuch, "Coupled-Cluster Method: An Accurate Ab Initio Theory of Atoms, Molecules, Nuclei, and Other Many-Fermion Systems," International Workshop on Microscopic Approaches to Nuclear Structure Calculations, UMIST, Manchester, U.K., July 4-8, 2004 [invited talk given by P. Piecuch].

- 115.\*\* P. Piecuch, "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Workshop "New Perspectives on p-Shell Nuclei," Michigan State University, East Lansing, U.S.A., July 22-24, 2004 [invited talk given by P. Piecuch].
- 116.\*\* P. Piecuch, K. Kowalski, I.S.O. Pimienta, M. J. McGuire, P.-D. Fan, and M. Lodriguito, "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," International conference "Molecular Quantum Mechanics: the No Nonsense Path to Progress" honoring Professor Nicholas Handy's work, St. John's College, Cambridge University, Cambridge, U.K., July 24-29, 2004 [invited talk given by P. Piecuch].
- 117.\*\* P. Piecuch, P.-D. Fan, S. Hirata, and K. Kowalski, "Renormalized Coupled-Cluster Methods and their Automated Parallel Computer Implementation with Tensor Contraction Engine," The symposium "Symbolic Calculation in Chemistry," 228th American Chemical Society National Meeting, Philadelphia, Pennsylvania, U.S.A., August 22-26, 2004 [invited talk given by P. Piecuch].
- 118.\*\* P. Piecuch, K. Kowalski, D.J. Dean, M. Hjorth-Jensen, T. Papenbrock, and M. Włoch, "Coupled Cluster Calculations of Ground and Excited States of Nuclei," International Conference on Exotic Nuclei and Atomic Masses, ENAM-04, Pine Mountain Georgia, September 12-16, 2004 [invited contributed talk given by P. Piecuch].
- 119.\*\* P. Piecuch, K. Kowalski, M. Włoch, and M. Lodriguito, "Non-Iterative Coupled-Cluster Methods For Accurate Calculations of Excited Electronic States," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004 [invited talk given by P. Piecuch].
- 120.\*\* P. Piecuch, M. Włoch, D.J. Dean, J.R. Gour, M. Hjorth-Jensen, K. Kowalski, and T. Papenbrock, "Coupled Cluster Calculations of Ground and Excited States of Nuclei," Ninth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-IX, Les Houches, Grenoble, France, September 25-30, 2004 [invited talk given by P. Piecuch].
- 121.\*\* P. Piecuch, "Coupled-Cluster Approaches to Atoms, Molecules, and Nuclei," Institute for Nuclear Theory workshop "Microscopic Nuclear Structure Theory," "Nuclear Forces and the Quantum Many-Body Problem," Seattle, Washington, U.S.A., October 4-8, 2004 [invited talk given by P. Piecuch].
- 122.\*\* M.D. Lodriguito, K. Kowalski, and P. Piecuch, "Method of Moments of Coupled-Cluster Equations Employing the Multireference Perturbation Theory," The symposium "Computational Chemical Dynamics from Gas-Phase to Condensed-Phase Systems," Minnesota Supercomputing Institute, University of Minnesota, Minneapolis, U.S.A., October 7-9, 2004 [poster presented by M. Lodriguito].
- 123.\*\* P. Piecuch, "Coupled-Cluster Method: Highly Accurate Microscopic Approach to Molecular Systems and Nuclei," Workshop "Nuclei and Mesoscopic Physics," Michigan State University, East Lansing, U.S.A., October 23-26, 2004 [invited talk given by P. Piecuch].
- 124.\*\* P. Piecuch, K. Kowalski, M. Włoch, J.R. Gour, M.J. McGuire, P.-D. Fan, A. Kinal, and M. Lodriguito, "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," 7th World Congress of Theoretically Oriented Chemists

- (WATOC05), Cape Town, South Africa, January 16-21, 2005. [invited talk given by P. Piecuch].
- 125.\*\* D.J. Dean, J.R. Gour, G. Hagen, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, P. Piecuch, and M. Włoch, "Challenges for Nuclear Structure: From Stable to Weakly Bound Nuclei," International Symposium on Correlation Dynamics in Nuclei – on the Occasion of the 50th Anniversary of the Configuration Mixing Theory of Arima and Horie, CDN05, Tokyo, Japan, January 31-February 4, 2005 [invited talk given by M. Hjorth-Jensen].
- 126.\*\* M.J. McGuire and P. Piecuch, "Renormalized Coupled-Cluster Studies of Reactions Involving Diradicals," the 45th Sanibel Symposium on Forefront Theory and Computation in Quantum Chemistry, Condensed Matter and Chemical Physics, Nanoscience, Quantum Biochemistry and Biophysics," St. Simons Island, Georgia, U.S.A., March 5-11, 2005 [poster presented by M.J. McGuire].
- 127.\*\* A. Kinal and P. Piecuch, "Is the Mechanism of Cycloaddition of Ethylene to Cyclopentene Concerted or Biradical? A Completely Renormalized Coupled Cluster Study," the 45th Sanibel Symposium on Forefront Theory and Computation in Quantum Chemistry, Condensed Matter and Chemical Physics, Nanoscience, Quantum Biochemistry and Biophysics," St. Simons Island, Georgia, U.S.A., March 5-11, 2005 [poster presented by A. Kinal].
- 128.\*\* M.D. Lodriguito, K. Kowalski, M. Włoch, and P. Piecuch, "Method of Moments of Coupled-Cluster Equations Employing the Multireference Perturbation Theory," the 45th Sanibel Symposium on Forefront Theory and Computation in Quantum Chemistry, Condensed Matter and Chemical Physics, Nanoscience, Quantum Biochemistry and Biophysics," St. Simons Island, Georgia, U.S.A., March 5-11, 2005 [poster presented by M. Lodriguito].
- 129.\*\* M. Włoch, J.R. Gour, K. Kowalski, and P. Piecuch, "The Open-Shell Extension of the Renormalized Equation of Motion Coupled-Cluster Method and its Applications to Many-Electron and Other Many-Fermion Systems," the 45th Sanibel Symposium on Forefront Theory and Computation in Quantum Chemistry, Condensed Matter and Chemical Physics, Nanoscience, Quantum Biochemistry and Biophysics," St. Simons Island, Georgia, U.S.A., March 5-11, 2005 [poster presented by M. Włoch].
- 130.\*\* K. Kowalski and P. Piecuch, "Extensive Generalization of Renormalized Coupled-Cluster Methods," the 45th Sanibel Symposium on Forefront Theory and Computation in Quantum Chemistry, Condensed Matter and Chemical Physics, Nanoscience, Quantum Biochemistry and Biophysics," St. Simons Island, Georgia, U.S.A., March 5-11, 2005 [invited talk given by K. Kowalski].
- 131.\*\* D.G. Truhlar, A.W. Jasper, S. Nangia, C. Zhu, P. Piecuch, and M.J. McGuire, "Quantum Photochemistry," John Pople Memorial Symposium, 229th American Chemical Society National Meeting, San Diego, California, U.S.A., March 13-17, 2005 [invited talk given by D.G. Truhlar].

- 132.\*\* P. Piecuch, M. Włoch, J.R. Gour, and K. Kowalski, "Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Electronic Quasi-Degeneracies and Open-Shell Problems," Fifth Congress of the International Society for Theoretical Chemical Physics (ICTCP-V), New Orleans, Louisiana, U.S.A., July 20-26, 2005 [invited plenary talk given by P. Piecuch].
- 133.\*\* M. Włoch, J.R. Gour, and P. Piecuch, "The Completely Renormalized Coupled-Cluster Approximations Exploiting the Right and Left Eigenstates of the Similarity-Transformed Hamiltonian," Fifth Congress of the International Society for Theoretical Chemical Physics (ICTCP-V), New Orleans, Louisiana, U.S.A., July 20-26, 2005 [poster presented by M. Włoch].
- 134.\*\* J.R. Gour, M. Włoch, and P. Piecuch, "The Active-Space Equation-of-Motion Coupled-Cluster Method for Electron-Attached and Ionized States," Fifth Congress of the International Society for Theoretical Chemical Physics (ICTCP-V), New Orleans, Louisiana, U.S.A., July 20-26, 2005 [poster presented by J.R. Gour].
- 135.\*\* S. Coussan, A. Trivella, C. Manca, Y. Ferro, M. Rajzmann, R. Wieczorek, P. Piecuch, K. Kowalski, M. Włoch, S.A. Kucharski, M. Musiał, and P. Roubin, "Acetylacetone Trapped in Inert Matrices: UV and IR Photo-Induced Isomerization and Theoretical Reactional Pathways," The conference "MATRIX-2005, The Physics and Chemistry of Matrix Isolated Species," Funchal, Portugal, July 24-29, 2005 [contributed talk given by S. Coussan].
- 136.\*\* P. Piecuch, M. Włoch, J.R. Gour, K. Kowalski, A. Kinal, M. Lodrigo, and M.J. McGuire, "Noniterative Coupled-Cluster Methods for Bond Breaking, Diradicals, and Excited Electronic States," The symposium "Theoretical Determination of Energy Landscapes: Methodology and Applications," 230th American Chemical Society National Meeting, Washington, DC, U.S.A., August 28-September 1, 2005. [invited talk given by P. Piecuch].
- 137.\*\* P. Piecuch, M. Włoch, and J.R. Gour, "Renormalized and Active-Space Coupled-Cluster Methods: Two Approaches to Quasi-Degeneracies and Open-Shell Problems," Conference on Microscopic Approaches to Many-Body Theory, in honor of Professor Raymond Bishop, The University of Manchester, Manchester, U.K., August 31-September 3, 2005 [invited talk given by P. Piecuch].
- 138.\*\* P. Piecuch, J.R. Gour, M. Włoch, and K. Kowalski, "Active-Space Coupled-Cluster Method: An Inexpensive and Highly Accurate Approach to Electronic Quasi-Degeneracies and Open-Shell Problems," Tenth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-X, Carthage, Tunisia, September 1-7, 2005 [invited talk given by P. Piecuch].
- 139.\*\* P. Piecuch, M. Włoch, and J.R. Gour, "Method of Moments of Coupled-Cluster Equations and Renormalized Coupled-Cluster Approaches to Bond Breaking: A Biorthogonal Size Extensive Formulation," Tenth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-X, Carthage, Tunisia, September 1-7, 2005 [poster presented by P. Piecuch].

- 140.\*\* P. Piecuch, M. Włoch, J.R. Gour, and A. Kinal, “Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems,” 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [invited talk given by P. Piecuch].
- 141.\*\* P. Piecuch and P.-D. Fan, “Intriguing Accuracies of the Exponential Wave Function Expansions Exploiting Finite Two-Body Correlation Operators in Calculations for Many-Electron Systems,” 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by P. Piecuch].
- 142.\*\* P. Piecuch, M. Włoch, J.R. Gour, D.J. Dean, T. Papenbrock, and M. Hjorth-Jensen, “Bridging Quantum Chemistry and Nuclear Structure Theory: Coupled-Cluster Calculations for Closed- and Open-Shell Nuclei,” 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by P. Piecuch].
- 143.\*\* J.R. Gour, P. Piecuch, and M. Włoch, “Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals,” 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by J.R. Gour].
- 144.\*\* Y. Ohtsuka, P. Piecuch, J.R. Gour, M. Ehara, and H. Nakatsuji, “Extension of the Active-Space Coupled-Cluster Methodology to the Symmetry-Adapted-Cluster Configuration-Interaction Approach,” 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by J.R. Gour].
- 145.\*\* M. Włoch, A. Kinal, J.R. Gour, and P. Piecuch, “Single-Reference, Size-Extensive, Non-Iterative Coupled-Cluster Approaches to Bond Breaking and Biradicals,” 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by M. Włoch].
- 146.\*\* M. Włoch and P. Piecuch, “Extension of Renormalized Coupled-Cluster Methods Including Triple Excitations to Ground and Excited Electronic States of Open-Shell Molecules,” 12th International Congress of Quantum Chemistry, Kyoto, Japan, May 21-26, 2006 [poster presented by M. Włoch].
- 147.\*\* M.D. Lodriguito, M. Włoch, and P. Piecuch, “Non-iterative Coupled-Cluster Methods Employing Multi-reference Perturbation Theory Wave Functions,” 38th Midwest Theoretical Chemistry Conference, Columbus, Ohio June 15-17, 2006 [poster presented by M.D. Lodriguito].
- 148.\*\* A. Kinal, M.J. McGuire, M. Włoch, and P. Piecuch, “Completely Renormalized Coupled-Cluster and Multi-Reference Configuration Interaction Studies of the Thermal Stereomutations of Cyclopropane,” 38th Midwest Theoretical Chemistry Conference, Columbus, Ohio June 15-17, 2006 [contributed talk given by A. Kinal].
- 149.\*\* P. Piecuch, “Accurate Quantum Calculations for Many-Electron and Other Many-Fermion Systems: From Bond Breaking and Electronic Excitations in Molecules to Properties of Atomic Nuclei,” The Centro Internacional de Matemática Workshop “Mathematics in Chemistry,” Lisbon, Portugal, July 19-21, 2006 [invited talk given by P. Piecuch].

- 150.\*\* P. Piecuch, M. Włoch, J.R. Gour, and A. Kinal, "Advances in Electronic Structure Theory: Single-Reference Coupled-Cluster Methods for Multi-Reference Problems," Sixth Canadian Computational Chemistry Conference (CCCC6), Vancouver, Canada, July 26-30, 2006 [invited plenary talk given by P. Piecuch].
- 151.\*\* M.D. Lodriguito, M. Włoch, and P. Piecuch, "Non-iterative Coupled-Cluster Methods Employing Multi-reference Perturbation Theory Wave Functions," Sixth Canadian Computational Chemistry Conference (CCCC6), Vancouver, Canada, July 26-30, 2006 [poster presented by M.D. Lodriguito].
- 152.\*\* P. Piecuch, M. Włoch, A. Kinal, and J.R. Gour, "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," Eleventh European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XI, St. Petersburg, Russia, August 20-25, 2006 [invited talk given by P. Piecuch].
- 153.\*\* P. Piecuch, M. Włoch, J.R. Gour, D.J. Dean, T. Papenbrock, and M. Hjorth-Jensen, "Bridging Quantum Chemistry and Nuclear Structure Theory: Coupled-Cluster Calculations for Closed- and Open-Shell Nuclei," Eleventh European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XI, St. Petersburg, Russia, August 20-25, 2006 [poster presented by P. Piecuch].
- 154.\*\* P. Piecuch, J.R. Gour, and M. Włoch, "Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals," Eleventh European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XI, St. Petersburg, Russia, August 20-25, 2006 [poster presented by P. Piecuch].
- 155.\*\* C. Sanz, O. Roncero, M.J. McGuire, and P. Piecuch, "Comparative study of the reactive collisions in CaHCl and BeHF systems," MOLEC XVI, European Conference on Dynamics of Molecular Systems, Levico Terme (Trento), Italy, September 11-15, 2006 [poster presented by C. Sanz].
- 156.\*\* P. Piecuch, "Accurate Quantum Calculations for Many-Body Systems: From Reaction Mechanisms in Organic and Bioinorganic Chemistries to Properties of Atomic Nuclei," Michigan State University High Performance Computing Center 2006 Symposium, East Lansing, Michigan, October 7, 2006 [invited talk].
- 157.\*\* P. Piecuch, M. Włoch, and J.R. Gour, "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," International Conference "Recent Trends in Many-Body Methods for Electronic Structure and Properties of Atoms and Molecules," Bhubaneswar and Puri, Orissa, India, January 11-13, 2007 [invited talk given by P. Piecuch].
- 158.\*\* P. Piecuch, J.R. Gour, and M. Włoch, "Active-Space Coupled-Cluster Methods for Bond Breaking, Excited Electronic States, and Open-Shell Systems," International Conference "Practicing Chemistry with Theoretical Tools, on the Occasion of Professor Mark S. Gordon's 65th Birthday," Kihei, Hawaii, U.S.A., January 15-18, 2007 [invited talk given by P. Piecuch].
- 159.\*\* M.D. Lodriguito and P. Piecuch, "Externally Corrected Coupled-Cluster Methods Employing Method of Moments of Coupled-Cluster Equations and Multi-Reference Perturbation Theory," 233rd American Chemical Society National Meeting, Chicago, Illinois,

- March 25-29 (2007) [poster presented by M.D. Lodriguito; Chemical Computing Group Graduate Student Excellence Award].
- 160.\*\* M. Horoi, J.R. Gour, M. Włoch, M.D. Lodriguito, P. Piecuch, and B.A. Brown, "Coupled-Cluster and Configuration-Interaction Calculations for Heavy Nuclei," Session X16, "Nuclear Theory II," 2007 American Physical Society April Meeting, Jacksonville, Florida, U.S.A., April 14-17, 2007 [talk given by M. Horoi].
- 161.\*\* P. Piecuch, M. Włoch, J.R. Gour, and A. Kinal "Advances in Electronic Structure Theory: Single-Reference Methods for Multi-Reference Problems," 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007 [invited talk given by P. Piecuch].
- 162.\*\* J.R. Gour and P. Piecuch, "Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals," 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007 [contributed talk given by J.R. Gour].
- 163.\*\* Y. Ohtsuka, P. Piecuch, J.R. Gour, M. Ehara, and H. Nakatsuji, "Extension of the Active-Space Coupled-Cluster Methodology to the Symmetry-Adapted-Cluster Configuration-Interaction Approach," 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007 [poster presented by J.R. Gour].
- 164.\*\* J.J. Lutz, P. Piecuch, and A. Kinal, "Extrapolating Potential Energy Surfaces for the Isomerization of Bicyclo[1.1.0]butane to Buta-1,3-diene," 39th Midwest Theoretical Chemistry Conference, Indiana University, Bloomington, Indiana, U.S.A., June 28-30, 2007 [poster presented by J.J. Lutz].
- 165.\*\* P. Piecuch, "Coupled-Cluster Theory: An Overview of the Basic Formalism and Applications to Molecular and Nuclear Structure Problems," Workshop on Advanced Many-body Methods for Nuclear Structure European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 2-6, 2007 [invited talk given by P. Piecuch].
- 166.\*\* P. Piecuch, M. Włoch, J.R. Gour, J.J. Lutz, and A. Kinal, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, and Bond Breaking," Twelfth European Workshop on Quantum Systems in Chemistry and Physics, QSCP-XII, London, U.K., August 30 - September 5, 2007 [invited talk given by P. Piecuch].
- 167.\*\* P. Piecuch, M. Włoch, J.R. Gour, J.J. Lutz, and A. Kinal, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Applications to Radicals, Biradicals, Reaction Pathways, and Photochemistry," "IXth International Conference on Molecular Spectroscopy: From Molecules to Molecular Biological Systems and Molecular Materials, Role of Molecular Interactions and Recognition," Wrocław – Łądek-Zdrój, Poland, September 13-18, 2007 [invited talk given by P. Piecuch].
- 168.\*\* J.R. Gour, M. Włoch, and P. Piecuch, in collaboration with B.A. Brown, D.J. Dean, M. Hjorth-Jensen, M. Horoi, T. Papenbrock, and R. Roth, "Bridging Quantum Chemistry

- and Nuclear Structure Theory: Coupled-Cluster Calculations for Closed- and Open-Shell Nuclei,” 2nd Workshop on Nuclei and Mesoscopic Physics, WNMP07, Michigan State University, East Lansing, Michigan, U.S.A., October 20-22, 2007 [poster presented by J.R. Gour].
- 169.\*\* J.R. Gour, P. Piecuch, and M. Włoch, “Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals,” 2nd Workshop on Nuclei and Mesoscopic Physics, WNMP07, Michigan State University, East Lansing, Michigan, U.S.A., October 20-22, 2007 [poster presented by J.R. Gour].
- 170.\*\* M. Włoch, J.R. Gour, A. Kinal, and P. Piecuch, “Single-Reference, Size-Extensive, Non-Iterative Coupled-Cluster Approaches to Bond Breaking and Biradicals,” 2nd Workshop on Nuclei and Mesoscopic Physics, WNMP07, Michigan State University, East Lansing, Michigan, U.S.A., October 20-22, 2007 [poster presented by J.R. Gour].
- 171.\*\* J.J. Lutz, P. Piecuch, and A. Kinal, “Extrapolating Potential Energy Surfaces for the Isomerization of Bicyclo[1.1.0]butane to Buta-1,3-diene,” 2nd Workshop on Nuclei and Mesoscopic Physics, WNMP07, Michigan State University, East Lansing, Michigan, U.S.A., October 20-22, 2007 [poster presented by J.J. Lutz].
- 172.\*\* K. Park, P. Piecuch, S.M. Bachrach, T. Nagata, K. Song, and W.L. Hase, “Direct Dynamics Study of the Atomic-Level Mechanism for the Reaction of Cyclopentyne with Ethylene,” 63rd Southwest Regional Meeting of the American Chemical Society, Lubbock, Texas, U.S.A., November 3-7, 2007 [poster contribution].
- 173.\*\* Y. Ge, M.S. Gordon, P. Piecuch, Marta Włoch, and J.R. Gour, “Breaking Bonds of Open-Shell Species with the Restricted Open-Shell Size Extensive Left Eigenstate Completely Renormalized Coupled-Cluster Method,” The symposium “Electronic Structure and Reaction Dynamics of Open-shell Species,” 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., April 6-10, 2008 [contributed talk given by Y. Ge].
- 174.\*\* P. Piecuch, M. Włoch, and J.R. Gour, “Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell Systems,” The symposium “Electronic Structure and Reaction Dynamics of Open-shell Species,” 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., April 6-10, 2008 [invited talk given by P. Piecuch].
- 175.\*\* J.R. Gour and P. Piecuch, “Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals and Other Open-Shell Species,” The symposium “Electronic Structure and Reaction Dynamics of Open-shell Species,” 235th American Chemical Society National Meeting, New Orleans, Louisiana, U.S.A., April 6-10, 2008 [poster given by J.R. Gour].
- 176.\*\* J.R. Gour, M. Horoi, P. Piecuch, and B.A. Brown, “Coupled-Cluster and Configuration-Interaction Calculations for Odd-A Heavy Nuclei,” The international conference “Nuclear Structure 2008” (NS2008), East Lansing, Michigan, U.S.A., June 3-6, 2008 [poster given by J.R. Gour].

- 177.\*\* J.J. Lutz, and P. Piecuch, "Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene," 40th Midwest Theoretical Chemistry Conference, University of Michigan, Ann Arbor, Michigan, U.S.A., June 26-28, 2008 [poster presented by J.J. Lutz].
- 178.\*\* W. Li, J.R. Gour, and P. Piecuch, "Local Correlation Calculations Using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods," 40th Midwest Theoretical Chemistry Conference, University of Michigan, Ann Arbor, Michigan, U.S.A., June 26-28, 2008 [poster presented by W. Li].
- 179.\*\* J.J. Lutz, and P. Piecuch, "Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene," Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, Michigan State University, East Lansing, Michigan, U.S.A., July 6-12, 2008 [poster presented by J.J. Lutz].
- 180.\*\* W. Li, J.R. Gour, and P. Piecuch, "Local Correlation Calculations Using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods," Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, Michigan State University, East Lansing, Michigan, U.S.A., July 6-12, 2008 [poster presented by W. Li].
- 181.\*\* J.R. Gour, P. Piecuch, and M. Ehara "Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals and Other Open-Shell Species," Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, Michigan State University, East Lansing, Michigan, U.S.A., July 6-12, 2008 [poster presented by J.R. Gour].
- 182.\*\* J.R. Gour, M. Włoch, and P. Piecuch, "Bridging Quantum Chemistry and Nuclear Structure Theory: Coupled-Cluster Calculations for Closed- and Open-Shell Nuclei," Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, Michigan State University, East Lansing, Michigan, U.S.A., July 6-12, 2008 [poster presented by J.R. Gour].
- 183.\*\* M. Włoch, P. Piecuch, and J.R. Gour, "Recent Developments and Applications of the Renormalized Coupled-Cluster Methods," Thirteenth International Workshop on Quantum Systems in Chemistry and Physics, Michigan State University, East Lansing, Michigan, U.S.A., July 6-12, 2008 [invited talk given by M. Włoch].
- 184.\*\* W. Li, J.R. Gour, and P. Piecuch, "Local Correlation Calculations Using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods," The 2008 American Conference on Theoretical Chemistry, Northwestern University, Evanston, Illinois, U.S.A., July 19-24, 2008 [poster presented by W. Li].
- 185.\*\* P. Piecuch, M. Włoch, J.R. Gour, and W. Li, "Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems," Sixth Congress of the International Society for Theoretical Chemical Physics (ICTCP-VI), Vancouver, British Columbia, Canada, July 19-24, 2008. [invited plenary talk given by P. Piecuch].
- 186.\*\* P. Piecuch, "Coupled-Cluster Theory: A Brief Overview of Modern Methods and Applications to Nuclear Structure," the WE-Heraeus-Seminar "Ab-Initio Nuclear Structure -

- Where do we stand?”, Bad Honnef, Germany, July 28-30, 2008 [invited talk given by P. Piecuch].
- 187.\*\* J.R. Gour, P. Piecuch, and M. Ehara, “Active-Space Equation-of-Motion Coupled-Cluster Methods for Ground and Excited States of Radicals and Other Open-Shell Systems,” Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008 [poster presented by J.R. Gour].
- 188.\*\* J.J. Lutz and P. Piecuch, “Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene,” Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008 [poster presented by J.J. Lutz].
- 189.\*\* P. Piecuch, M. Włoch, J.R. Gour, and W. Li, “Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems,” 8th World Congress of Theoretically Oriented Chemists (WATOC08), Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008 [invited lecture given by P. Piecuch].
- 190.\*\* W. Li, P. Piecuch, and J.R. Gour, “Local Correlation Calculations Using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods,” 8th World Congress of Theoretically Oriented Chemists (WATOC08), Eighth Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC 2008), Sydney, Australia, September 14-19, 2008 [poster presented by P. Piecuch].
- 191.\*\* P. Piecuch, W. Li, J.R. Gour, and M. Włoch, “Renormalized Coupled-Cluster Methods: Theoretical Foundations and Extension to Open-Shell and Large Systems,” The International Conference on the Theory and Applications of Computational Chemistry in 2008 (TACC 2008), Shanghai, China, September 23-27, 2008 [invited plenary lecture given by P. Piecuch].
- 192.\*\* J.J. Lutz and P. Piecuch, “Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene,” Symposium to Honor Professor Peter Wagner in Celebration of his Career and 70th Birthday, Michigan State University, East Lansing, Michigan, U.S.A., October 10-11, 2008 [poster presented by J.J. Lutz].
- 193.\*\* W. Li, P. Piecuch, and J.R. Gour, “Local Correlation Calculations Using Cluster-In-Molecule Standard and Renormalized Coupled-Cluster Methods,” Symposium to Honor Professor Peter Wagner in Celebration of his Career and 70th Birthday, Michigan State University, East Lansing, Michigan, U.S.A., October 10-11, 2008 [poster presented by W. Li].
- 194.\*\* P. Piecuch, W. Li, and J.R. Gour, “Local Correlation Calculations Using Standard and Renormalized Coupled-Cluster Methods,” Focus Session “The Chemical Physics of Biological and Biologically-Inspired Solar Energy Harvesting III,” the 2009 American Physical Society March Meeting, Pittsburgh, Pennsylvania, U.S.A., March 16-20, 2009 [associated with the award of Fellowship of APS; contributed talk given by P. Piecuch].

- 195.\*\* P. Piecuch, W. Li, J.J. Lutz, and J.R. Gour, "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," The symposium "Advances in Electronic Structure Theory and First Principles Dynamics," 237th American Chemical Society National Meeting, Salt Lake City, Utah, U.S.A., March 22-26, 2009 [invited talk given by P. Piecuch].
- 196.\*\* P. Piecuch, "New Single- and Multi-Reference Coupled-Cluster Methods for High Accuracy Calculations of Ground and Excited States," 30th Annual Combustion Research Meeting, Airlie Conference Center, Warrenton, Virginia, May 26-29, 2009 [invited talk given by P. Piecuch].
- 197.\*\* M. Włoch, P. Piecuch, and J.R. Gour, "Recent Developments and Applications of the Renormalized Coupled-Cluster Methods," 92nd Canadian Chemistry Conference and Exhibition, Hamilton, Ontario, Canada, May 30 - June 3, 2009 [invited talk given by M. Włoch].
- 198.\*\* P. Piecuch, "Coupled-Cluster Theory: From Quantum Chemistry to Applications in Nuclear Physics," International Workshop "Linking Nuclei, Molecules, and Condensed Matter: Computational Quantum Many-Body Approaches," European Centre for Theoretical Studies in Nuclear Physics and Related Areas, Trento, Italy, July 6-10, 2009 [invited talk given by P. Piecuch].
- 199.\*\* P. Piecuch, J.R. Gour, W. Li, M. Włoch, and K. Kowalski, "Dealing with Strong Electron Correlations in Quantum Chemistry via Renormalized, Active-Space, and Multi-Reference Coupled-Cluster Methods," The symposium "New Developments in Strongly Correlated Electrons," 238th American Chemical Society National Meeting, Washington, DC, U.S.A., August 16-20, 2009 [invited talk given by P. Piecuch].
- 200.\*\* P. Piecuch, W. Li, J.J. Lutz, and J.R. Gour, "Extending Electronic Structure Theory to Complex Molecular Problems: Local Correlation Coupled-Cluster and Correlation Energy Scaling Methodologies," Fourteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XIV, San Lorenzo del Escorial, Madrid, Spain, September 13-19, 2009 [invited talk to be given by P. Piecuch].
- 201.\*\* J.R. Gour and P. Piecuch, "Active-Space Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methods," Fourteenth International Workshop on Quantum Systems in Chemistry and Physics, QSCP-XIV, San Lorenzo del Escorial, Madrid, Spain, September 13-19, 2009 [invited talk to be given by J.R. Gour].
- 202.\*\* TBA, International conference on "Recent Advances in Many-Electron Theories," Raman Center for the Atomic, Molecular, and Optical Sciences, Indian Association for the Cultivation of Science, Kolkata, India, January 4-6, 2010 [invited talk to be given by P. Piecuch].
- 203.\*\* P. Piecuch, TBA, 10-minute perspective talk preceding a session on multi-reference coupled-cluster theory, the 50th Sanibel Symposium, St. Simons Island, Georgia, U.S.A., February 24-March 2, 2010 [to be given].
- 204.\*\* TBA, International conference "Molecular Quantum Mechanics: From Methylene to DNA and Beyond" honoring Professor Henry F. Schaefer's work, University of California at Berkeley, Berkeley, California, May 24-29, 2010 [invited talk to be given by P. Piecuch].