

LIST OF PIOTR PIECUCH'S PUBLICATIONS[†]

1. Monographs, Book Chapters, and Feature Articles^{††}

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 Electronic 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, Vol. 5*, edited by J. Leszczynski (World Scientific, Singapore, 2000), 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. Dyll (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].

[†] 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 **. Clickable hyperlinks to listed publications are marked by blue color.

^{††} All other invited papers are listed with the remaining original articles.

- 8.** P. Piecuch, K. Kowalski, P.-D. Fan, and I.S.O. Pimienta, “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. 89-97 [invited book chapter].
- 13.** T. Papenbrock, D.J. Dean, J.R. Gour, G. Hagen, M. Hjorth-Jensen, P. Piecuch, and M. Włoch, “Coupled-Cluster Theory for Nuclei,” in: *Recent Progress in Many-Body Theories, Vol. 10*, edited by S. Hernández and H. Cataldo (World Scientific, Singapore, 2006), pp. 385-392 [invited book chapter].
- 14.** 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, Dordrecht, 2006), pp. 45-106 [invited advanced review book chapter].
- 15.** 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].
- 16.** 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, Dordrecht, 2007), pp. 63-121 [invited book chapter].

- 17.** 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].
- 18.** 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].
- 19.** 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, Dordrecht, 2008), pp. 67-174 [invited book chapter].
- 20.** 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 Institute of Physics, Melville, NY, 2009), pp. 68-113 [invited book chapter in conference proceedings].
- 21.** 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, Dordrecht, 2009), pp. 131-195 [invited book chapter].
- 22.** G. Fradelos, J.J. Lutz, T.A. Wesolowski, P. Piecuch, and M. Włoch "Shifts in Excitation Energies Induced by Hydrogen Bonding: A Comparison of the Embedding and Supermolecular Time-Dependent Density Functional Theory Calculations with the Equation-of-Motion Coupled-Cluster Results," in: *Progress in Theoretical Chemistry and Physics, Vol. 22*, "Advances in the Theory of Quantum Systems in Chemistry and Physics," edited by P.E. Hoggan, E. Brändas, J. Maruani, P. Piecuch, and G. Delgado-Barrio (Springer, Dordrecht, 2012), pp. 219-248 [invited book chapter].
- 23.** P. Piecuch, M. Włoch, J.R. Gour, W. Li, and J.J. Lutz, "Dealing with Chemical Reaction Pathways and Electronic Excitations in Molecular Systems via Renormalized and Active-Space Coupled-Cluster Methods," in: *Proceedings of the International Conference on Computational Methods in Science and Engineering 2010 (ICCMSE-2010), AIP Conference Proceedings, Vol. 1642*, edited by T.E. Simos and G. Maroulis (AIP Publishing, Melville, NY, 2015), pp. 172-175 [invited article in conference proceedings].

2. Articles

24. P. Piecuch, "Invariance Properties of the Multipole Expansion," *Int. J. Quantum Chem.* **22**, 293-298 (1982).
25. P. Piecuch, "Spherical Tensor Theory of Long-Range Interactions between Two Molecules," *Int. J. Quantum Chem.* **25**, 449-473 (1984).
26. 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).
27. P. Piecuch, "Spherical Multipole Moments and Polarizabilities of Tetrahedral and Octahedral Molecules," *Acta Phys. Pol. A* **66**, 69-80 (1984).
28. 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).
29. M.M. Szczyński, 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).
30. P. Piecuch, "Note on the Multipole Expansion in the Spherical Tensor Form," *J. Phys. A: Math. Gen.* **18**, L739-L743 (1985).
31. P. Piecuch, "Supplement to Spherical Tensor Theory of Long-Range Interactions between Two Molecules," *Int. J. Quantum Chem.* **28**, 375-386 (1985).
32. 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).
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34. 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).
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36. P. Piecuch, "On the Addition Theorems for Solid Spherical Harmonics," *Rep. Math. Phys.* **24**, 187-192 (1986).
37. 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).

38. 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).
39. 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).
40. 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).
41. 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).
42. 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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45. 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) or *Int. J. Quantum Chem.* **40**, Issue Supplement S25, 9-34 (1991).
46. J. Paldus and P. Piecuch, "Electron Correlation in One Dimension: Coupled Cluster Approaches to Cyclic Polyene π -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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54. P. Piecuch and J. Paldus, "Application of Hilbert-Space Coupled-Cluster Theory to Simple (H₂)₂ Model Systems. II. Non-Planar Models," *Phys. Rev. A* **49**, 3479-3514 (1994).
55. P. Piecuch and L. Adamowicz, "State-Selective Multireference Coupled-Cluster Theory Employing the Single-Reference Formalism: Implementation and Application to the H₈ Model System," *J. Chem. Phys.* **100**, 5792-5809 (1994).
56. P. Piecuch and L. Adamowicz, "Solving the Single-Reference Coupled-Cluster Equations Involving Highly Excited Clusters in Quasidegenerate Situations," *J. Chem. Phys.* **100**, 5857-5869 (1994).
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58. X. Li, P. Piecuch, and J. Paldus, "A Study of ¹A₁ – ³B₁ Separation in CH₂ Using Orthogonally Spin-Adapted State-Universal and State-Specific Coupled-Cluster Methods," *Chem. Phys. Lett.* **224**, 267-274 (1994).
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60. P. Piecuch, X. Li, and J. Paldus, "An *Ab Initio* Determination of ¹A₁ – ³B₁ Energy Gap in CH₂ Using Orthogonally Spin-Adapted State-Universal and State-Specific Coupled-Cluster Methods," *Chem. Phys. Lett.* **230**, 377-386 (1994).
61. 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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74. P. Piecuch, "Potential Energy Curves for the HF⁻ and CH₃F⁻ 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].
75. X.Y. Chang, R. Ehlich, A.J. Hudson, P. Piecuch, and J.C. Polanyi, "Dynamics of Harpooning Studied by Transition State Spectroscopy. Na⋯FH," *Faraday Discuss. Chem. Soc.* **108**, 411-425 (1997) [in response to an invitation issued to J.C. Polanyi].
76. X.Y. Chang, A.J. Hudson, P. Piecuch, and J.C. Polanyi, "Communication on REMPI Two-Photon Ionization Experiment for NaF," included in *General Discussion* published as *Faraday Discuss. Chem. Soc.* **108**, 427-467 (1997); see the communication by A.J. Hudson and J.C. Polanyi on pp. 463-464.

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- 86.* K. Kowalski and P. Piecuch, "Complete Set of Solutions of Multi-Reference Coupled-Cluster Equations: The State-Universal Formalism," *Phys. Rev. A* **61**, 052506-1 - 052506-8 (2000).
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LIST OF JOURNAL ISSUES AND BOOKS EDITED BY PIOTR PIECUCH

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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3. *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). Preface: p. vii.
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