

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 Multi-molecular 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. Dyall (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 Chemican 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. Wesołowski, 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. Szczęśniak, 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).
33. 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).
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).
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52. P. Piecuch, N. Oliphant, and L. Adamowicz, "A State-Selective Multi-Reference Coupled-Cluster Theory Employing the Single-Reference Formalism," *J. Chem. Phys.* **99**, 1875-1900 (1993).
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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).
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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 Multireference Coupled-Cluster Method Employing the Single-Reference Formalism," *J. Chem. Phys.* **102**, 898-904 (1995).
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63. P. Piecuch, R. Toboła, 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,” *Int. J. Quantum Chem.* **55**, 133-146 (1995).
64. A.E. Kondo, P. Piecuch, and J. Paldus, “Orthogonally Spin-Adapted Single-Reference Coupled-Cluster Formalism: Linear Response Calculation of Static Properties,” *J. Chem. Phys.* **102**, 6511-6524 (1995).
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 75. X.Y. Chang, R. Ehlich, A.J. Hudson, P. Piecuch, and J.C. Polanyi, “Dynamics of Harpooning Studied by Transition State Spectroscopy. Na \cdots FH,” *Faraday Discuss.* **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.* **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).
2. *Progress in Theoretical Chemistry and Physics* (book series published by Springer), Volume 18 (2008), “Frontiers in Quantum Systems in Chemistry and Physics.” Proceedings from the Twelfth European Workshop on Quantum Systems in Chemistry and Physics (London, U.K., August 30 - September 5, 2007). Edited by S. Wilson, P. Grout, J. Maruani, G. Delgado-Barrio, and P. Piecuch. Preface: pp. vii-viii.
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.
4. *Progress in Theoretical Chemistry and Physics* (book series published by Springer), Volume 19 (2009), “Advances in the Theory of Atomic and Molecular Systems: Conceptual and Computational Advances in Quantum Chemistry.” 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. Preface: pp. vii-ix.
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