

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. 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].

[†] 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).
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).
35. 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).
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).
43. P. Piecuch, S. Zarrabian, J. Paldus, and J. Čížek, "Coupled-Cluster Approaches with an Approximate Account of Triexcitations and the Optimized-Inner-Projection Technique. III. Lower Bounds to the Ground-State Correlation Energy of Cyclic-Polyene Model Systems," *Phys. Rev. A* **42**, 5155-5167 (1990).
44. K. Jankowski, J. Paldus, and P. Piecuch, "Method of Moments Approach and Coupled Cluster Theory," *Theor. Chim. Acta* **80**, 223-243 (1991).
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"].
47. P. Piecuch, J. Čížek, and J. Paldus, "Behavior of Coupled Cluster Energy in the Strongly Correlated Limit of the Cyclic Polyene Model. Comparison with the Exact Results," *Int. J. Quantum Chem.* **42**, 165-191 (1992) [invited paper in a special issue devoted to "Hartree-Fock-Based Correlation Treatments of Extended Systems"].
48. P. Piecuch and J. Paldus, "Orthogonally Spin-Adapted Multi-Reference Hilbert Space Coupled-Cluster Formalism: Diagrammatic Formulation," *Theor. Chim. Acta* **83**, 69-103 (1992) [invited paper in the Klaus Ruedenberg honorary issue].
49. J. Paldus, P. Piecuch, L. Pylypow, and B. Jeziorski, "Application of Hilbert-Space Coupled-Cluster Theory to Simple $(H_2)_2$ Model Systems: Planar Models," *Phys. Rev. A* **47**, 2738-2782 (1993).

50. 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).
51. P. Piecuch, R. Tobiła, and J. Paldus, "Approximate Account of Connected Quadruply Excited Clusters in Multi-Reference Hilbert Space Coupled Cluster Theory: Application to Planar H₄ Models," *Chem. Phys. Lett.* **210**, 243-252 (1993).
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).
53. M.M. Szcześniak, G. Chałasiński, and P. Piecuch, "The Non-Additive Interactions in the Ar₂HF and Ar₂HCl Clusters: An *Ab Initio* Study," *J. Chem. Phys.* **99**, 6732-6741 (1993).
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).
57. P. Piecuch and L. Adamowicz, "State-Selective Multi-Reference Coupled-Cluster Theory Using Multi-Configuration Self-Consistent-Field Orbitals. A Model Study on H₈," *Chem. Phys. Lett.* **221**, 121-128 (1994).
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).
59. 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).
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).
62. V. Alexandrov, P. Piecuch, and L. Adamowicz, "State-Selective Multi-Reference Coupled-Cluster Theory Employing the Single-Reference Formalism: Application to an Excited State of H₈," *J. Chem. Phys.* **102**, 3301-3306 (1995).
63. P. Piecuch, R. Tobiła, 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).
65. P. Piecuch and J. Paldus, "Property Evaluation Using the Two-Reference State-Universal Coupled-Cluster Method," *J. Phys. Chem.* **99**, 15354-15368 (1995) [invited contribution, Zdenek Herman Festschrift].
66. 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).
67. P. Piecuch, A.E. Kondo, V. Špirko, and J. Paldus, "Molecular Quadrupole Moment Functions of HF and N₂. I. *Ab Initio* Linear-Response Coupled-Cluster Results," *J. Chem. Phys.* **104**, 4699-4715 (1996).
68. V. Špirko, P. Piecuch, A.E. Kondo, and J. Paldus, "Molecular Quadrupole Moment Functions of HF and N₂. II. Rovibrational Effects," *J. Chem. Phys.* **104**, 4716-4727 (1996).
69. K.B. Ghose, P. Piecuch, S. Pal, and L. Adamowicz, "State-Selective Multi-Reference Coupled-Cluster Theory: In Pursuit of Property Calculation," *J. Chem. Phys.* **104**, 6582-6589 (1996).
70. A.E. Kondo, P. Piecuch, and J. Paldus, "Orthogonally Spin-Adapted Single-Reference Coupled-Cluster Formalism: Linear Response Calculation of Higher-Order Static Properties," *J. Chem. Phys.* **104**, 8566-8585 (1996).
71. P. Piecuch, R. Toboła, and J. Paldus, "Approximate Account of Connected Quadruply Excited Clusters in Single-Reference Coupled-Cluster Theory via Cluster Analysis of the Projected Unrestricted Hartree-Fock Wave Function," *Phys. Rev. A* **54**, 1210-1241 (1996).
72. P. Piecuch, V. Špirko, and J. Paldus, "Molecular Quadrupole Moment Function of Ammonia," *J. Chem. Phys.* **105**, 11068-11074 (1996).
73. 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).
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.

77. P. Piecuch, V. Špirko, A.E. Kondo, and J. Paldus, "Vibrational Dependence of the Dipole Moment and Radiative Transition Probabilities in the $X^1\Sigma^+$ State of HF: A Linear-Response Coupled-Cluster Study," *Mol. Phys.* **94**, 55-64 (1998) [invited contribution; in response to an invitation issued to P. Piecuch].
78. L. Adamowicz, P. Piecuch, and K.B. Ghose, "The State-Selective Coupled Cluster Method for Quasidegenerate Electronic States," *Mol. Phys.* **94**, 225-234 (1998) [invited contribution; in response to an invitation issued to L. Adamowicz].
79. P. Piecuch, V. Špirko, and J. Paldus, "Dipole Moment and Polarizability Functions of Ammonia: A Linear-Response Coupled-Cluster Study," *Pol. J. Chem.* **72** (7S), 1635-1656 (1998) [invited contribution in a special issue dedicated to late Włodzimierz Kolos; edited by B. Jeziorski and L. Piela; in response to an invitation issued to P. Piecuch].
80. M.S. Topaler, D.G. Truhlar, X.Y. Chang, P. Piecuch, and J.C. Polanyi, "Potential Energy Surfaces of NaFH," *J. Chem. Phys.* **108**, 5349-5377 (1998).
81. M.S. Topaler, D.G. Truhlar, X.Y. Chang, P. Piecuch, and J.C. Polanyi, "The Photoabsorption Spectrum of Na \cdots FH van der Waals Molecule: Comparison of Theory and Experiment for a Harpooning Reaction Studied by Transition State Spectroscopy," *J. Chem. Phys.* **108**, 5378-5390 (1998).
82. 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," *J. Chem. Phys.* **110**, 6103-6122 (1999).
- 83.* M.S. Topaler, P. Piecuch, and D.G. Truhlar, "Infrared Absorption Line Strengths of the Na \cdots FH van der Waals Molecule," *J. Chem. Phys.* **110**, 5634-5638 (1999).
- 84.* 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," *J. Chem. Phys.* **111**, 6679-6692 (1999).
- 85.* V. Špirko, P. Piecuch, and O. Bludsky, "Bound and Quasi-Bound States of the Na \cdots FH van der Waals Molecule," *J. Chem. Phys.* **112**, 189-202 (2000).
- 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).
- 87.* K. Kowalski and P. Piecuch, "The Method of Moments of Coupled-Cluster Equations and the Renormalized CCSD[T], CCSD(T), CCSD(TQ), and CCSDT(Q) Approaches," *J. Chem. Phys.* **113**, 18-35 (2000).
- 88.* P. Piecuch and J.I. Landman, "Parallelization of Multi-Reference Coupled-Cluster Method," *Parallel Comp.* **26**, 913-943 (2000) [the *Computational Chemistry* issue of *Parallel Computing*; invited paper; in response to an invitation issued to P. Piecuch].
- 89.* K. Kowalski and P. Piecuch, "Renormalized CCSD(T) and CCSD(TQ) Approaches: Dissociation of the N₂ Triple Bond," *J. Chem. Phys.* **113**, 5644-5652 (2000).
- 90.* K. Kowalski and P. Piecuch, "The Active-Space Equation-of-Motion Coupled-Cluster Methods for Excited Electronic States: The EOMCCSDt Approach," *J. Chem. Phys.* **113**, 8490-8502 (2000).

- 91.* S. Šekusak, P. Piecuch, R.J. Bartlett, and M.G. Cory, "A General Reaction Path Dual-Level Direct Dynamics Calculation of the Reaction of Hydroxyl Radical with Dimethyl Sulfide," *J. Phys. Chem. A* **104**, 8779-8786 (2000).
- 92.* F. Mrugała, P. Piecuch, V. Špirko, and O. Bludsky, "Lifetimes and Dissociation Pathways of Quasi-Bound States of the $\text{Na}\cdots\text{FH}$ van der Waals Molecule," *J. Molec. Struct.* **555**, 43-60 (2000) [invited paper; in response to an invitation issued to P. Piecuch].
- 93.* K. Kowalski and P. Piecuch, "Complete Set of Solutions of the Generalized Bloch Equation," *Int. J. Quantum Chem.* **80**, 757-781 (2000) [Special Issue: Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory, edited by N.Y. Öhrn and J.R. Sabin].
- 94.* 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," *Int. J. Quantum Chem.* **80**, 916-933 (2000) [Special Issue: Proceedings of the International Symposium on Atomic, Molecular, and Condensed Matter Theory, edited by N.Y. Öhrn and J.R. Sabin].
- 95.* A.J. Hudson, H.B. Oh, J.C. Polanyi, and P. Piecuch, "Dynamics of Harpooning Studied by Transition State Spectroscopy. II. $\text{Li}\cdots\text{FH}$," *J. Chem. Phys.* **113**, 9897-9900 (2000).
- 96.* J.I. Landman and P. Piecuch, "Parallelization of a Legacy Research Program Using OpenMP," *Fortran Forum* **19**, 16-23 (2000).
- 97.* K. Kowalski and P. Piecuch, "The State-Universal Multi-Reference Coupled-Cluster Theory with Perturbative Description of Core-Virtual Excitations," *Chem. Phys. Lett.* **334**, 89-98 (2001).
- 98.* A.K. Füžery, R. Burcl, L.L. Torday, P. Császár, O. Farkas, A. Perczel, M.A. Zamora, J.G. Papp, B. Penke, P. Piecuch, and I.G. Csizmadia, "Can NO_2^+ Exist in Bent or Cyclic Forms?," *Chem. Phys. Lett.* **334**, 381-386 (2001).
- 99.* K. Kowalski and P. Piecuch, "Extension of the Method of Moments of Coupled-Cluster Equations to a Multireference Wave Operator Formalism," *J. Molec. Struct.: THEOCHEM* **547**, 191-208 (2001) [invited paper in a special issue of *THEOCHEM* in honor of Professor Josef Paldus entitled "Electron Correlation;" edited by A.J. Thakkar and C.E. Dykstra; in response to an invitation issued to P. Piecuch].
- 100.* K. Kowalski and P. Piecuch, "The Active-Space Equation-of-Motion Coupled-Cluster Methods for Excited Electronic States: Full EOMCCSDt," *J. Chem. Phys.* **115**, 643-651 (2001).
- 101.* K. Kowalski and P. Piecuch, "A Comparison of the Renormalized and Active-Space Coupled-Cluster Methods: Potential Energy Curves of BH and F_2 ," *Chem. Phys. Lett.* **344**, 165-175 (2001).
- 102.* P. Piecuch, S.A. Kucharski, and K. Kowalski, "Can Ordinary Single-Reference Coupled-Cluster Methods Describe the Potential Energy Curve of N_2 ? The Renormalized CCSDT(Q) Study," *Chem. Phys. Lett.* **344**, 176-184 (2001).
- 103.* K. Kowalski and P. Piecuch, "New Type of the Noniterative Energy Correction for Excited Electronic States: Extension of the Method of Moments of Coupled-Cluster Equations to Equation-of-Motion Coupled-Cluster Formalism," *J. Chem. Phys.* **115**, 2966-2978 (2001).

- 104.* P. Piecuch, S.A. Kucharski, V. Špirko, and K. Kowalski, "Can Ordinary Single-Reference Coupled-Cluster Methods Describe Potential Energy Surfaces with Nearly Spectroscopic Accuracy? The Renormalized Coupled-Cluster Study of the Vibrational Spectrum of HF," *J. Chem. Phys.* **115**, 5796-5804 (2001).
- 105.* A.W. Jasper, M.D. Hack, A. Chakraborty, D.G. Truhlar, and P. Piecuch, "Photodissociation of LiFH and NaFH van der Waals Complexes: A Semiclassical Trajectory Study," *J. Chem. Phys.* **115**, 7945-7952 (2001); *J. Chem. Phys.* **119**, 9321 (2003) [Erratum].
- 106.* K. Kowalski and P. Piecuch, "Excited-State Potential Energy Curves of CH⁺: A Comparison of the EOMCCSDt and Full EOMCCSDT Results," *Chem. Phys. Lett.* **347**, 237-246 (2001).
- 107.* A.W. Jasper, M.D. Hack, D.G. Truhlar, and P. Piecuch, "Coupled Quasidiabatic Potential Energy Surfaces for LiFH," *J. Chem. Phys.* **116**, 8353-8366 (2002).
- 108.** K. Kowalski and P. Piecuch, "Extension of the Method of Moments of Coupled-Cluster Equations to Excited States: The Triples and Quadruples Corrections to the Equation-of-Motion Coupled-Cluster Singles and Doubles Energies," *J. Chem. Phys.* **116**, 7411-7423 (2002).
- 109.** P. Piecuch, K. Kowalski, and I.S.O. Pimienta, "Method of Moments of Coupled-Cluster Equations: Externally Corrected Approaches Employing Configuration Interaction Wave Functions," *Int. J. Mol. Sci.* **3**, 475-497 (2002) [invited paper; in response to an invitation issued to P. Piecuch].
- 110.** P. Piecuch and K. Kowalski, "The State-Universal Multi-Reference Coupled-Cluster Theory: An Overview of Some Recent Advances," *Int. J. Mol. Sci.* **3**, 676-709 (2002) [invited paper; in response to an invitation issued to P. Piecuch].
- 111.** R. Burcl, P. Piecuch, V. Špirko, and O. Bludsky, "Bound and Quasi-Bound States of the Li...FH van der Waals Molecule: The Effect of the Potential Energy Surface and of the Basis Set Superposition Error," *J. Molec. Struct.: THEOCHEM* **591**, 151-174 (2002) [invited paper in a special issue of *THEOCHEM* in honor of Professor William Meath entitled "Intermolecular Forces;" edited by A.J. Thakkar; in response to an invitation issued to P. Piecuch].
- 112.** M.J. McGuire, K. Kowalski, and P. Piecuch, "Renormalized Coupled-Cluster Calculations of Reactive Potential Energy Surfaces: A Comparison of the CCSD(T), Renormalized CCSD(T), and Full CI Results for the Collinear BeFH System," *J. Chem. Phys.* **117**, 3617-3624 (2002).
- 113.** P. Piecuch, S.A. Kucharski, K. Kowalski, and M. Musiał, "Efficient Computer Implementation of the Renormalized Coupled-Cluster Methods: The R-CCSD[T], R-CCSD(T), CR-CCSD[T], and CR-CCSD(T) Approaches," *Comp. Phys. Commun.* **149**, 71-96 (2002).
- 114.** P. Piecuch, K. Kowalski, P.-D. Fan, and K. Jedziniak, "Exactness of Two-Body Cluster Expansions in Many-Body Quantum Theory," *Phys. Rev. Lett.* **90**, 113001-1 - 113001-4 (2003).
- 115.** I.S.O. Pimienta, K. Kowalski, and P. Piecuch, "Method of Moments of Coupled-Cluster Equations: The Quasi-Variational and Quadratic Approximations," *J. Chem. Phys.* **119**, 2951-2962 (2003).

- 116.** K. Kowalski and P. Piecuch, "New Coupled-Cluster Methods with Singles, Doubles, and Noniterative Triples for High Accuracy Calculations of Excited Electronic States," *J. Chem. Phys.* **120**, 1715-1738 (2004).
- 117.** R.L. DeKock, M.J. McGuire, P. Piecuch, W.D. Allen, H.F. Schaefer III, K. Kowalski, S.A. Kucharski, M. Musiał, A.R. Bonner, S.A. Spronk, D.B. Lawson, and S.L. Laursen, "The Electronic Structure and Vibrational Spectrum of trans-HNOO," *J. Phys. Chem. A* **108**, 2893-2903 (2004) [Henry F. Schaefer III Festschrift, invited contribution].
- 118.** K. Kowalski, D.J. Dean, M. Hjorth-Jensen, T. Papenbrock, and P. Piecuch, "Coupled Cluster Calculations of Ground and Excited States of Nuclei," *Phys. Rev. Lett.* **92**, 132501-1 – 132501-4 (2004).
- 119.** M.J. McGuire, P. Piecuch, K. Kowalski, S.A. Kucharski, and M. Musiał, "Renormalized Coupled-Cluster Calculations of Reactive Potential Energy Surfaces: The BeFH System," *J. Phys. Chem. A* **108**, 8878-8893 (2004) [the Gert D. Billing Festschrift, invited contribution, in response to an invitation issued to P. Piecuch].
- 120.** K. Kowalski and P. Piecuch, "New Classes of Noniterative Energy Corrections to Multi-Reference Coupled-Cluster Energies," *Mol. Phys.* **102**, 2425-2449 (2004) [special issue in honor of Professor Nicholas C. Handy; edited by H.F. Schaefer III; invited contribution, in response to an invitation issued to P. Piecuch].
- 121.** S. Hirata, P.-D. Fan, A.A. Auer, M. Nooijen, and P. Piecuch, "Combined Coupled-Cluster and Many-Body Perturbation Theories," *J. Chem. Phys.* **121**, 12197–12207 (2004).
- 122.** R.M. Olson, S. Varganov, M.S. Gordon, H. Metiu, S. Chretien, P. Piecuch, K. Kowalski, S.A. Kucharski, and M. Musiał, "Where Does the Planar-to-Nonplanar Turnover Occur in Small Gold Clusters?," *J. Am. Chem. Soc.* **127**, 1049-1052 (2005).
- 123.** M.J. McGuire and P. Piecuch, "Balancing Dynamic and Non-Dynamic Correlation for Diradical and Aromatic Transition States: A Renormalized Coupled-Cluster Study of the Cope Rearrangement of 1,5-Hexadiene," *J. Am. Chem. Soc.* **127**, 2608-2614 (2005).
- 124.** K. Kowalski and P. Piecuch, "Extensive Generalization of Renormalized Coupled-Cluster Methods," *J. Chem. Phys.* **122**, 074107-1–074107-12 (2005).
- 125.** C.D. Sherrill and P. Piecuch, "The $X^1\Sigma_g^+$, $B^1\Delta_g$, and $B'^1\Sigma_g^+$ States of C_2 : A Comparison of Renormalized Coupled-Cluster and Multireference Methods with Full Configuration Interaction Benchmarks," *J. Chem. Phys.* **122**, 124104-1–124104-17 (2005).
- 126.** R.K. Chaudhuri, K.F. Freed, G. Hose, P. Piecuch, K. Kowalski, M. Włoch, S. Chattopadhyay, D. Mukherjee, Z. Rolik, Á. Szabados, G. Tóth, and P.R. Surján, "Comparison of Low-Order Multireference Many-Body Perturbation Theories," *J. Chem. Phys.* **122**, 134105-1–134105-9 (2005).
- 127.** D.J. Dean, J.R. Gour, G. Hagen, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, P. Piecuch, and M. Włoch, "Nuclear Structure Calculations with Coupled Cluster Methods from Quantum Chemistry," *Nucl. Phys. A* **752**, 299-308 (2005) [Special

- Issue: Proceedings of the 22nd International Nuclear Physics Conference, Goeteborg, Sweden; edited by B. Jonson, M. Meister, G. Nyman, and M. Zhukov].
- 128.** P.-D. Fan, K. Kowalski, and P. Piecuch, "Noniterative Corrections to Extended Coupled-Cluster Energies Employing the Generalized Method of Moments of Coupled-Cluster Equations," *Mol. Phys.* **103**, 2191-2213 (2005) [special issue in honor of Professor Rodney J. Bartlett; edited by J.F. Stanton; invited contribution, in response to an invitation issued to P. Piecuch].
 - 129.** M. Włoch, J.R. Gour, K. Kowalski, and P. Piecuch, "Extension of Renormalized Coupled-Cluster Methods Including Triple Excitations to Excited Electronic States of Open-Shell Molecules," *J. Chem. Phys.* **122**, 214107-1 – 214107-15 (2005).
 - 130.** M. Włoch, D.J. Dean, J.R. Gour, P. Piecuch, M. Hjorth-Jensen, T. Papenbrock, and K. Kowalski, "Ab Initio Coupled-Cluster Calculations for Nuclei Using Methods of Quantum Chemistry," *Eur. Phys. J. A* **25** (Suppl. 1), 485-488 (2005) (*Eur. Phys. J. A Direct*; electronic only) [Special Issue: Proceedings of the International Conference on Exotic Nuclei and Atomic Masses, ENAM-04; edited by C. Gross, W. Nazarewicz, and K. Rykaczewski].
 - 131.** M. Włoch, J.R. Gour, P. Piecuch, D.J. Dean, M. Hjorth-Jensen, and T. Papenbrock, "Coupled-Cluster Calculations for Ground and Excited States of Closed- and Open-Shell Nuclei Using Methods of Quantum Chemistry," *J. Phys. G: Nucl. Part. Phys.* **31**, S1291-S1299 (2005) [special issue dedicated to the workshop "Nuclear Forces and the Quantum Many-Body Problem," edited by D.J. Dean, B.R. Barrett, M. Hjorth-Jensen, and J.P. Vary; invited contribution, in response to an invitation issued to P. Piecuch].
 - 132.** M. Włoch, D.J. Dean, J.R. Gour, M. Hjorth-Jensen, K. Kowalski, T. Papenbrock, and P. Piecuch, "Ab Initio Coupled-Cluster Study of ^{16}O ," *Phys. Rev. Lett.* **94**, 212501-1–212501-4 (2005).
 - 133.** K. Kowalski, S. Hirata, M. Włoch, P. Piecuch, and T.L. Windus, "Active-Space Coupled-Cluster Study of Electronic States of Be_3 ," *J. Chem. Phys.* **123**, 074319-1–074319-6 (2005).
 - 134.** J.R. Gour, P. Piecuch, and M. Włoch, "Active-Space Equation-of-Motion Coupled-Cluster Methods for Excited States of Radicals and Other Open-Shell Systems: EA-EOMCCSDt and IP-EOMCCSDt," *J. Chem. Phys.* **123**, 134113-1–134113-14 (2005).
 - 135.** P. Piecuch and M. Włoch, "Renormalized Coupled-Cluster Methods Exploiting Left Eigenstates of the Similarity-Transformed Hamiltonian," *J. Chem. Phys.* **123**, 224105-1–224105-10 (2005).
 - 136.** S. Nangia, D.G. Truhlar, M.J. McGuire, and P. Piecuch, "Can a Single-Reference Approach Provide a Balanced Description of Ground and Excited States? A Comparison of the Completely Renormalized Equation-of-Motion Coupled-Cluster Method with Multi-Reference Quasi-Degenerate Perturbation Theory Near a Conical Intersection and Along a Photodissociation Coordinate in Ammonia," *J. Phys. Chem. A* **109**, 11643-11646 (2005).
 - 137.** P. Piecuch, M. Włoch, J.R. Gour, and A. Kinal, "Single-Reference, Size-Extensive, Non-Iterative Coupled-Cluster Approaches to Bond Breaking and Biradicals," *Chem. Phys. Lett.* **418**, 467-474 (2006); published online on November 28, 2005.

- 138.** P. Piecuch, S. Hirata, K. Kowalski, P.-D. Fan, and T.L. Windus, "Automated Derivation and Parallel Computer Implementation of Renormalized and Active-Space Coupled-Cluster Methods," *Int. J. Quantum Chem.* **106**, 79-97 (2006) [Special Issue: Mathematical Methods and Symbolic Calculation in Chemistry and Chemical Biology; edited by M.P. Barnett and F.E. Harris; invited contribution, in response to an invitation issued to P. Piecuch].
- 139.** A. Kinal and P. Piecuch, "Is the Mechanism of the [2+2] Cycloaddition of Cyclopentyne to Ethylene Concerted or Biradical? A Completely Renormalized Coupled Cluster Study," *J. Phys. Chem. A* **110**, 367-378 (2006) [special issue in honor of Professor Donald G. Truhlar, invited contribution, in response to an invitation issued to P. Piecuch].
- 140.** C.J. Cramer, M. Włoch, P. Piecuch, C. Puzzarini, and L. Gagliardi, "Theoretical Models on the Cu₂O₂ Torture Track. Mechanistic Implications for Oxytyrosinase and Small-Molecule Analogues," *J. Phys. Chem. A* **110**, 1991-2004 (2006); *ibid.* **111**, 4871-4871 (2007) [Addition/Correction].
- 141.** S. Coussan, Y. Ferro, A. Trivella, M. Rajzmann, P. Roubin, R. Wieczorek, C. Manca, P. Piecuch, K. Kowalski, M. Włoch, S.A. Kucharski, and M. Musiał, "Experimental and Theoretical UV Characterizations of Acetylacetone and its Isomers," *J. Phys. Chem. A* **110**, 3920-3926 (2006).
- 142.** M. Włoch, M.D. Lodriguito, P. Piecuch, and J.R. Gour, "Two New Classes of Non-Iterative Coupled-Cluster Methods Derived from the Method of Moments of Coupled-Cluster Equations," *Mol. Phys.* **104**, 2149-2172 (2006); *Mol. Phys.* **104**, 2991 (2006) [Erratum; last name of Włoch corrected] [special issue in honor of Professor Andrzej J. Sadlej, invited contribution, in response to an invitation issued to P. Piecuch].
- 143.** J.R. Gour, P. Piecuch, M. Hjorth-Jensen, M. Włoch, and D.J. Dean, "Coupled-Cluster Calculations for Valence Systems around ¹⁶O," *Phys. Rev. C* **74**, 024310-1-024310-18 (2006).
- 144.** J.R. Gour, P. Piecuch, and M. Włoch, "Extension of the Active-Space Equation-of-Motion Coupled-Cluster Methods to Radical Systems: The EA-EOMCCSDt and IP-EOMCCSDt Approaches," *Int. J. Quantum Chem.* **106**, 2854-2874 (2006) [special issue dedicated to the proceedings of the Fifth Congress of the International Society for Theoretical Chemical Physics (ISTCP-V), edited by P. Politzer, J. Murray, and E. Brändas].
- 145.** M.D. Lodriguito, K. Kowalski, M. Włoch, and P. Piecuch, "Non-Iterative Coupled-Cluster Methods Employing Multi-Reference Perturbation Theory Wave Functions," *J. Mol. Struct: THEOCHEM* **771**, 89-104 (2006) [the WATOC 2005 special issue, edited by K.J. Naidoo, H.F. Schaefer III, T. Ford, E.D. Jemmis, and G. Frenking; invited contribution, in response to an invitation issued to P. Piecuch].
- 146.** P.-D. Fan and P. Piecuch, "Intriguing Accuracies of the Exponential Wave Function Expansions Exploiting Finite Two-Body Correlation Operators in Calculations for Many-Electron Systems," *J. Mol. Struct: THEOCHEM* **768**, 3-16 (2006) [special issue in honor of Professor Debashis Mukherjee, invited contribution, in response to an invitation issued to P. Piecuch].

- 147.** A.J.C. Varandas and P. Piecuch, "Extrapolating Potential Energy Surfaces by Scaling Electron Correlation at a Single Geometry," *Chem. Phys. Lett.* **430**, 448-453 (2006).
- 148.** C.J. Cramer, A. Kinal, M. Włoch, P. Piecuch, and L. Gagliardi, "Theoretical Characterization of End-on and Side-on Peroxide Coordination in Ligated Cu_2O_2 Models," *J. Phys. Chem. A* **110**, 11557-11568 (2006); *ibid.* **111**, 4871-4871 (2007) [Addition/Correction].
- 149.** J.R. Gour and P. Piecuch, "Efficient Formulation and Computer Implementation of the Active-Space Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methods," *J. Chem. Phys.* **125**, 234107-1 – 234107-17 (2006).
- 150.** T. Papenbrock, D.J. Dean, J.R. Gour, G. Hagen, M. Hjorth-Jensen, P. Piecuch, and M. Włoch, "Coupled Cluster Theory for Nuclei," *Int. J. Mod. Phys. B* **20** (Nos. 30-31), 5338-5345 (2006) [special issue dedicated to the 13th International Conference on Recent Progress in Many-Body Theories, edited by S. Hernández and H. Cataldo, invited contribution].
- 151.** A. Kinal and P. Piecuch, "Computational Investigation of the Conrotatory and Disrotatory Isomerization Channels of Bicyclo[1.1.0]butane to Buta-1,3-diene: A Completely Renormalized Coupled-Cluster Study," *J. Phys. Chem. A* **111**, 734-742 (2007).
- 152.** M. Horoi, J.R. Gour, M. Włoch, M.D. Lodriguito, B.A. Brown, and P. Piecuch, "Coupled-Cluster and Configuration-Interaction Calculations for Heavy Nuclei," *Phys. Rev. Lett.* **98**, 112501-1 – 112501-4 (2007).
- 153.** Y. Ohtsuka, P. Piecuch, J.R. Gour, M. Ehara, and H. Nakatsuji, "Active-Space Symmetry-Adapted-Cluster Configuration-Interaction and Equation-of-Motion Coupled-Cluster Methods for High Accuracy Calculations of Potential Energy Surfaces of Radicals," *J. Chem. Phys.* **126**, 164111-1 – 164111-28 (2007).
- 154.** M. Włoch, J.R. Gour, and P. Piecuch, "Extension of the Renormalized Coupled-Cluster Methods Exploiting Left Eigenstates of the Similarity-Transformed Hamiltonian to Open-Shell Systems: A Benchmark Study," *J. Phys. Chem. A* **111**, 11359 -11382 (2007) [special issue in honor of Professor Thom H. Dunning, Jr., invited contribution, in response to an invitation issued to P. Piecuch].
- 155.** G. Hagen, T. Papenbrock, D.J. Dean, A. Schwenk, A. Nogga, M. Włoch, and P. Piecuch, "Coupled-Cluster Theory for Three-Body Hamiltonians," *Phys. Rev. C* **76**, 034302-1 - 034302-11 (2007).
- 156.** Y. Ge, M.S. Gordon, and P. Piecuch, "Breaking Bonds with the Left Eigenstate Completely Renormalized Coupled-Cluster Method," *J. Chem. Phys.* **127**, 174106-1 - 174106-6 (2007).
- 157.** P. Piecuch, M. Włoch, and A.J.C. Varandas, "Application of Renormalized Coupled-Cluster Methods to Potential Function of Water," *Theor. Chem. Acc.* **120**, 59-78 (2008); published online on May 15, 2007 [special issue in honor of Professor Mark S. Gordon, invited contribution, in response to an invitation issued to P. Piecuch].
- 158.** J. Zheng, J.R. Gour, J.J. Lutz, M. Włoch, P. Piecuch, and D.G. Truhlar, "A Comparative Assessment of the Perturbative and Renormalized Coupled Cluster Theories with a Non-iterative Treatment of Triple Excitations for Thermochemical

- Kinetics, Including a Study of Basis Set and Core Correlation Effects,” *J. Chem. Phys.* **128**, 044108-1 – 044108-7 (2008).
- 159.** C.J. Cramer, J.R. Gour, A. Kinal, M. Włoch, P. Piecuch, A.R.M. Shahi, and L. Gagliardi, “Stereo-electronic Effects on Molecular Geometries and State-Energy Splittings of Ligated Monocopper Dioxygen Complexes,” *J. Phys. Chem. A* **112**, 3754-3767 (2008).
- 160.** J.J. Lutz and P. Piecuch, “Extrapolating Potential Energy Surfaces by Scaling Electron Correlation: Isomerization of Bicyclobutane to Butadiene,” *J. Chem. Phys.* **128**, 154116-1 – 154116-12 (2008).
- 161.** Y.Z. Song, A. Kinal, P.J.S.B. Caridade, A.J.C. Varandas, and P. Piecuch, “A Comparison of Single-Reference Coupled-Cluster and Multi-Reference Configuration Interaction Methods for Representative Cuts of the $\text{H}_2\text{S}(^1A')$ Potential Energy Surface,” *J. Mol. Struct: THEOCHEM* **859**, 22-29 (2008).
- 162.** P. Piecuch, J.R. Gour, and M. Włoch, “Biorthogonal Method of Moments of Coupled-Cluster Equations: Alternative Derivation, Further Considerations, and Application to a Model Magnetic System,” *Int. J. Quantum Chem.* **108**, 2128-2149 (2008) [special issue in honor of Professor Karol Jankowski; edited by L. Meissner and I. Grabowski; invited contribution, in response to an invitation issued to P. Piecuch].
- 163.** J.R. Gour, M. Horoi, P. Piecuch, and B.A. Brown, “Coupled-Cluster and Configuration-Interaction Calculations for Odd-A Heavy Nuclei,” *Phys. Rev. Lett.* **101**, 052501-1 – 052501-4 (2008).
- 164.** X. Li, J.R. Gour, J. Paldus, and P. Piecuch, “On the Significance of Quadruply Excited Clusters in Coupled-Cluster Calculations for the Low-Lying States of BN and C_2 ,” *Chem. Phys. Lett.* **461**, 321-326 (2008).
- 165.** Y. Ge, M.S. Gordon, P. Piecuch, M. 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,” *J. Phys. Chem. A* **112**, 11873-11884 (2008).
- 166.** R. Roth, J.R. Gour, and P. Piecuch, “*Ab Initio* Coupled-Cluster and Configuration Interaction Calculations for ^{16}O Using the V_{UCOM} Interaction,” *Phys. Rev. C* **79**, 054325-1 – 054325-19 (2009).
- 167.** Y. Zhao, O. Tishchenko, J.R. Gour, W. Li, J.J. Lutz, P. Piecuch, and D.G. Truhlar, “Thermochemical Kinetics for Multireference Systems: Addition Reactions of Ozone,” *J. Phys. Chem. A* **113**, 5786-5799 (2009).
- 168.** M. Ehara, J.R. Gour, and P. Piecuch, “Low-Lying Valence Excited States of CNC, C_2N , N_3 , and NCO Studied Using the Electron-Attached and Ionized Symmetry-Adapted-Cluster Configuration-Interaction and Equation-of-Motion Coupled-Cluster Methodologies,” *Mol. Phys.* **107**, 871-880 (2009) [special issue in honor of Professor Henry F. Schaefer, III; edited by T.D. Crawford and C.D. Sherrill; invited contribution, in response to an invitation issued to P. Piecuch].
- 169.** J. Pittner and P. Piecuch, “Method of Moments for the Continuous Transition Between the Brillouin-Wigner-Type and Rayleigh-Schrödinger-Type Multireference Coupled Cluster Theories,” *Mol. Phys.* **107**, 1209-1221 (2009) [special issue in

- honor of Professor Henry F. Schaefer, III; edited by T.D. Crawford and C.D. Sherrill; invited contribution].
- 170.** P. Piecuch, J.R. Gour, and M. Włoch, “Left-Eigenstate Completely Renormalized Equation-of-Motion Coupled-Cluster Methods: Review of Key Concepts, Extension to Excited States of Open-Shell Systems, and Comparison with Electron-Attached and Ionized Approaches,” *Int. J. Quantum Chem.* **109**, 3268-3304 (2009) [special issue dedicated to the proceedings of the Sixth Congress of the International Society for Theoretical Chemical Physics (ISTCP-VI), edited by Y.A. Wang, E. Brändas, and J. Maruani].
- 171.** R. Roth, J.R. Gour, and P. Piecuch, “Center-of-Mass Problem in Truncated Configuration Interaction and Coupled-Cluster Calculations,” *Phys. Lett. B* **679**, 334-339 (2009).
- 172.** W. Li, P. Piecuch, J.R. Gour, and S. Li, “Local Correlation Calculations Using Standard and Renormalized Coupled-Cluster Approaches,” *J. Chem. Phys.* **131**, 114109-1 – 114109-30 (2009).
- 173.** W. Li and P. Piecuch, “Multilevel Extension of the Cluster-in-Molecule Local Correlation Methodology: Merging Coupled-Cluster and Møller-Plesset Perturbation Theories,” *J. Phys. Chem. A* **114**, 6721-6727 (2010).
- 174.** W. Li and P. Piecuch, “Improved Design of Orbital Domains within the Cluster-in-Molecule Local Correlation Framework: Single-Environment Cluster-in-Molecule Ansatz and its Application to Local Coupled-Cluster Approach with Singles and Doubles,” *J. Phys. Chem. A* **114**, 8644-8657 (2010) [special issue in honor of Professor Klaus Ruedenberg, invited contribution, in response to an invitation issued to P. Piecuch].
- 175.** P. Arora, W. Li, P. Piecuch, J.W. Evans, M. Albao, and M.S. Gordon, “Diffusion of Atomic Oxygen on the Si(100) Surface,” *J. Phys. Chem. C* **114**, 12649-12658 (2010).
- 176.** J.R. Gour, P. Piecuch, and M. Włoch, “Comparison of the Completely Renormalized Equation-of-Motion Coupled-Cluster and Quantum Monte Carlo Results for the Low-Lying Electronic States of Methylene,” *Mol. Phys.* **108**, 2633-2646 (2010) [special issue entitled “Proceedings of Molecular Quantum Mechanics 2010: An International Conference in Honour of Professor Henry F. Schaefer III”; invited contribution, in response to an invitation issued to P. Piecuch].
- 177.** P. Piecuch, “Active-Space Coupled-Cluster Methods,” *Mol. Phys.* **108**, 2987-3015 (2010) [special issue entitled “Electrons, Molecules, Solids, and Biosystems: Fifty Years of the Quantum Theory Project”; invited contribution].
- 178.** G. Fradelos, J.J. Lutz, T.A. Wesolowski, P. Piecuch, and M. Włoch, “Embedding vs Supermolecular Strategies in Evaluating the Hydrogen-Bonding-Induced Shifts of Excitation Energies,” *J. Chem. Theory Comput.* **7**, 1647-1666 (2011).
- 179.** J.A. Hansen, P. Piecuch, J.J. Lutz, and J.R. Gour, “Geometries and Adiabatic Excitation Energies of the Low-Lying Valence States of CNC, C₂N, N₃, and NCO Studied with the Electron-Attached and Ionized Equation-of-Motion Coupled-Cluster Methodologies,” *Phys. Scr.* **84**, 028110 (2011) (17pp) [special CAMOP-Molec2010 issue of *Physica Scripta* dedicated to the 18th European Conference on Dynamics of Molecular Systems (MOLEC-XVIII); invited contribution].

- 180.** M. Ehara, P. Piecuch, J.J. Lutz, and J.R. Gour, "Symmetry-Adapted-Cluster Configuration-Interaction and Equation-of-Motion Coupled-Cluster Studies of Electronically Excited States of Copper Tetrachloride and Copper Tetrabromide Dianions," *Chem. Phys.* **399**, 94-110 (2012) [special issue "New Trends in Atomic and Molecular Clusters" in honor of Professor Gerardo Delgado-Barrio; invited contribution, in response to an invitation issued to P. Piecuch].
- 181.** G.R. Magoon, J. Aguilera-Iparraguirre, W.H. Green, J.J. Lutz, P. Piecuch, H.-W. Wong, and O.O. Oluwole, "Detailed Chemical Modeling of JP-10 (*exo*-tetrahydrodicyclopentadiene) High Temperature Oxidation: Exploring the Role of Biradical Species in Initial Decomposition Steps," *Int. J. Chem. Kin.* **44**, 179-193 (2012).
- 182.** J. Shen and P. Piecuch, "Biorthogonal Moment Expansions in Coupled-Cluster Theory: Review of Key Concepts and Merging the Renormalized and Active-Space Coupled-Cluster Methods," *Chem. Phys.* **401**, 180-202 (2012) [special issue "Recent Advances in Electron Correlation Methods and Applications" in honor of Professor Debashis Mukherjee; invited contribution, in response to an invitation issued to P. Piecuch].
- 183.** J. Shen and P. Piecuch, "Combining Active-Space Coupled-Cluster Methods with Moment Energy Corrections via the $CC(P;Q)$ Methodology, with Benchmark Calculations for Biradical Transition States," *J. Chem. Phys.* **136**, 144104-1 – 144104-16 (2012).
- 184.** S.A. Nedd, N.J. De Yonker, A.K. Wilson, P. Piecuch, and M.S. Gordon, "Incorporating a Completely Renormalized Coupled Cluster Approach into a Composite Method for Thermodynamic Properties and Reaction Paths," *J. Chem. Phys.* **136**, 144109-1 – 144109-13 (2012).
- 185.** P.M. Kozłowski, M. Kumar, P. Piecuch, W. Li, N.P. Bauman, J.A. Hansen, P. Lodowski, and M. Jaworska, "The Cobalt-Methyl Bond Dissociation in Methylcobalamin: New Benchmark Analysis Based on Density Functional Theory and Completely Renormalized Coupled-Cluster Calculations," *J. Chem. Theory Comput.* **8**, 1870-1894 (2012).
- 186.** J. Shen and P. Piecuch, "Merging Active-Space and Renormalized Coupled-Cluster Methods via the $CC(P;Q)$ Formalism, with Benchmark Calculations for Singlet-Triplet Gaps in Biradical Systems," *J. Chem. Theory Comput.* **8**, 4968-4988 (2012) [special issue in honor of Professor H. Bernhard Schlegel, invited contribution, in response to an invitation issued to P. Piecuch].
- 187.** K. Kornobis, N. Kumar, P. Lodowski, M. Jaworska, P. Piecuch, J.J. Lutz, B.M. Wong, and P.M. Kozłowski, "Electronic Structure of the S_1 State in Methylcobalamin: Insight from CASSCF/MC-XQDPT2, EOM-CCSD, and TD-DFT Calculations," *J. Comp. Chem.* **34**, 987-1004 (2013).
- 188.** J. Shen and P. Piecuch, "Doubly Electron-Attached and Doubly Ionized Equation-of-Motion Coupled-Cluster Methods with 4-particle–2-hole and 4-hole–2-particle Excitations and their Active-Space Extensions," *J. Chem. Phys.* **138**, 194102-1 – 194102-16 (2013).
- 189.** P. Piecuch, J.A. Hansen, D. Staedter, S. Faure, and V. Blanchet, "Communication: Existence of the Doubly Excited State that Mediates the Photoionization of

- Azulene,” *J. Chem. Phys.* **138**, 201102-1 – 201102-4 (2013).
- 190.** J.A. Hansen, P. Piecuch, and B.G. Levine, “Communication: Determining the Lowest-Energy Isomer of Au₈: 2D, or not 2D,” *J. Chem. Phys.* **139**, 091101-1 – 091101-4 (2013).
- 191.** J.A. Hansen, M. Ehara, and P. Piecuch, “Aerobic Oxidation of Methanol to Formic Acid on Au₈⁻: Benchmark Analysis Based on Completely Renormalized Coupled-Cluster and Density Functional Theory Calculations,” *J. Phys. Chem. A* **117**, 10416-10427 (2013).
- 192.** C.E.P. Bernardo, N.P. Bauman, P. Piecuch, and P.J. Silva, “Evaluation of Density Functional Methods on the Geometric and Energetic Descriptions of Species Involved in Cu⁺-Promoted Catalysis,” *J. Mol. Model.* **19**, 5457-5467 (2013).
- 193.** S. Binder, P. Piecuch, A. Calci, J. Langhammer, P. Navrátil, and R. Roth, “Extension of Coupled-Cluster Theory with a Non-iterative Treatment of Connected Triply Excited Clusters to Three-Body Hamiltonians,” *Phys. Rev. C* **88**, 054319-1 – 054319-21 (2013).
- 194.** J. Shen and P. Piecuch, “Doubly Electron-Attached and Doubly Ionised Equation-of-Motion Coupled-Cluster Methods with Full and Active-Space Treatments of 4-particle-2-hole and 4-hole-2-particle Excitations: The Role of Orbital Choices,” *Mol. Phys.* **112**, 868-885 (2014) [special issue entitled “Proceedings of Molecular Quantum Mechanics 2013: An International Conference in Honour of Professor Rodney J. Bartlett”; invited contribution, in response to an invitation issued to P. Piecuch].
- 195.** J.J. Lutz and P. Piecuch, “Performance of the Completely Renormalized Equation-of-Motion Coupled-Cluster Method in Calculations of Excited-State Potential Cuts of Water,” *Comput. Theor. Chem.* **1040-1041**, 20-34 (2014) [special issue entitled “Excited States: From Isolated Molecules to Complex Environments”; invited contribution, in response to an invitation issued to P. Piecuch].
- 196.** N.P. Bauman, J.A. Hansen, M. Ehara, and P. Piecuch, “Communication: Coupled-Cluster Interpretation of the Photoelectron Spectrum of Au₃⁻,” *J. Chem. Phys.* **141**, 101102-1 – 101102-5 (2014).
- 197.** P. Piecuch, J.A. Hansen, and A.O. Ajala, “Benchmarking the Completely Renormalised Equation-of-Motion Coupled-Cluster Approaches for Vertical Excitation Energies,” *Mol. Phys.* **113**, 3085-3127 (2015) [Special Issue in Honour of Professor Sourav Pal; invited contribution, in response to an invitation issued to P. Piecuch].
- 198.** J.A. Hansen, N.P. Bauman, J. Shen, W.T. Borden, and P. Piecuch, “*Ab Initio* Coupled-Cluster and Multi-Reference Configuration Interaction Studies of the Low-Lying Electronic States of 1,2,3,4-Cyclobutanetetraone,” *Mol. Phys.* **114**, 695-708 (2016); published online: 9 December 2015.
- 199.** K. Duanmu, O. Roberto-Neto, F.B.C. Machado, J.A. Hansen, J. Shen, P. Piecuch, and D.G. Truhlar, “Geometries, Binding Energies, Ionization Potentials, and Electron Affinities of Metal Clusters: Mg_n^{0,±1}, n = 1 – 7,” *J. Phys. Chem. C* **120**, 13275-13286 (2016).
- 200.** N.P. Bauman, J.A. Hansen, and P. Piecuch, “Coupled-Cluster Interpretation of the Photoelectron Spectrum of Ag₃⁻,” *J. Chem. Phys.* **145**, 084306-1 – 084306-9 (2016).

- 201.** G. Rasskazov, M. Nairat, I. Magoulas, V.V. Lozovoy, P. Piecuch, and M. Dantus, "Femtosecond Real-Time Probing of Reactions MMXVII: The Predissociation of Sodium Iodide in the A 0^+ State," *Chem. Phys. Lett.* **683**, 121-127 (2017) [the Zewail Memorial Issue; invited contribution, in response to an invitation issued to M. Dantus].
- 202.** A.O. Ajala, J. Shen, and P. Piecuch, "Economical Doubly Electron-Attached Equation-of-Motion Coupled-Cluster Methods with an Active-Space Treatment of Three-Particle–One-Hole and Four-Particle–Two-Hole Excitations," *J. Phys. Chem. A* **121**, 3469-3485 (2017) [special issue in honor of Professor Mark S. Gordon, invited contribution, in response to an invitation issued to P. Piecuch].
- 203.** N.P. Bauman, J. Shen, and P. Piecuch, "Combining Active-Space Coupled-Cluster Approaches with Moment Energy Corrections via the CC($P;Q$) Methodology: Connected Quadruple Excitations," *Mol. Phys.* **115**, 2860-2891 (2017) [Special Issue in Honour of Professor Debashis Mukherjee; invited contribution, in response to an invitation issued to P. Piecuch].
- 204.** E. Pastorczak, J. Shen, M. Hapka, P. Piecuch, and K. Pernal, "Intricacies of van der Waals Interactions in Systems with Elongated Bonds Revealed by Electron-Groups Embedding and High-Level Coupled-Cluster Approaches," *J. Chem. Theory Comput.* **13**, 5404-5419 (2017).
- 205.** S.J. Stoneburner, J. Shen, A.O. Ajala, P. Piecuch, D.G. Truhlar, and L. Gagliardi, "Systematic Design of Active Spaces for Multi-Reference Calculations of Singlet–Triplet Gaps of Organic Diradicals, with Benchmarks against Doubly Electron-Attached Coupled-Cluster Data," *J. Chem. Phys.* **147**, 164120-1 – 164120-12 (2017).
- 206.** J.E. Deustua, J. Shen, and P. Piecuch, "Converging High-Level Coupled-Cluster Energetics by Monte Carlo Sampling and Moment Expansions," *Phys. Rev. Lett.* **119**, 223003-1 – 223003-5 (2017).
- 207.** I. Magoulas, N.P. Bauman, J. Shen, and P. Piecuch, "Application of the CC($P;Q$) Hierarchy of Coupled-Cluster Methods to the Beryllium Dimer," *J. Phys. Chem. A* **122**, 1350-1368 (2018) [special issue in honor of Professors Manuel Yáñez and Otilia Mó, invited contribution, in response to an invitation issued to P. Piecuch].
- 208.** J.E. Deustua, I. Magoulas, J. Shen, and P. Piecuch, "Communication: Approaching Exact Quantum Chemistry by Cluster Analysis of Full Configuration Interaction Quantum Monte Carlo Wave Functions," *J. Chem. Phys.* **149**, 151101-1 – 151101-6 (2018).
- 209.** S.H. Yuwono, I. Magoulas, J. Shen, and P. Piecuch, "Application of the Coupled-Cluster CC($P;Q$) Approaches to the Magnesium Dimer," *Mol. Phys.*, in press; published online: 8 January, 2019 [Special Memorial Issue in Honour of Professor Dieter Cremer; invited contribution, in response to an invitation issued to P. Piecuch].

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.
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. Preface: pp. vii-ix.
6. *International Journal of Quantum Chemistry*, Volume 111, Issue 2 (2011). Special Issue: Proceedings from the Fourteenth European Workshop on Quantum Systems in Chemistry and Physics (San Lorenzo de El Escorial, Madrid, Spain, September 13-19, 2009). Issue Edited by Gerardo Delgado-Barrio, Jean Maruani, Piotr Piecuch, and Erkki Brändas. Preface: *Int. J. Quantum Chem.* **111** (2), 203-204 (2011). List of Participants: *Int. J. Quantum Chem.* **111** (2), 205-212 (2011).
7. *Progress in Theoretical Chemistry and Physics* (book series published by Springer), Volume 22 (2012), "Advances in the Theory of Quantum Systems in Chemistry and Physics." Proceedings from the Fifteenth International Workshop on Quantum Systems in Chemistry and Physics (Cambridge, U.K., August 31 - September 5, 2010). Edited by P.E. Hoggan, E. Brändas, J. Maruani, P. Piecuch, and G. Delgado-Barrio. Preface: pp. xv-xvii.
8. *Progress in Theoretical Chemistry and Physics* (book series published by Springer), Volume 26 (2012), "Quantum Systems in Chemistry and Physics: Progress in Methods and

Applications.” Proceedings from the Sixteenth International Workshop on Quantum Systems in Chemistry and Physics (Kanazawa, Japan, September 11-17, 2011). Edited by K. Nishikawa, J. Maruani, E. Brändas, G. Delgado-Barrio, and P. Piecuch. [Preface](#): pp. vii-ix.